

STC Center for Integrated Quantum Materials  
2013-2014 Center Overview  
NSF DMR-1231319

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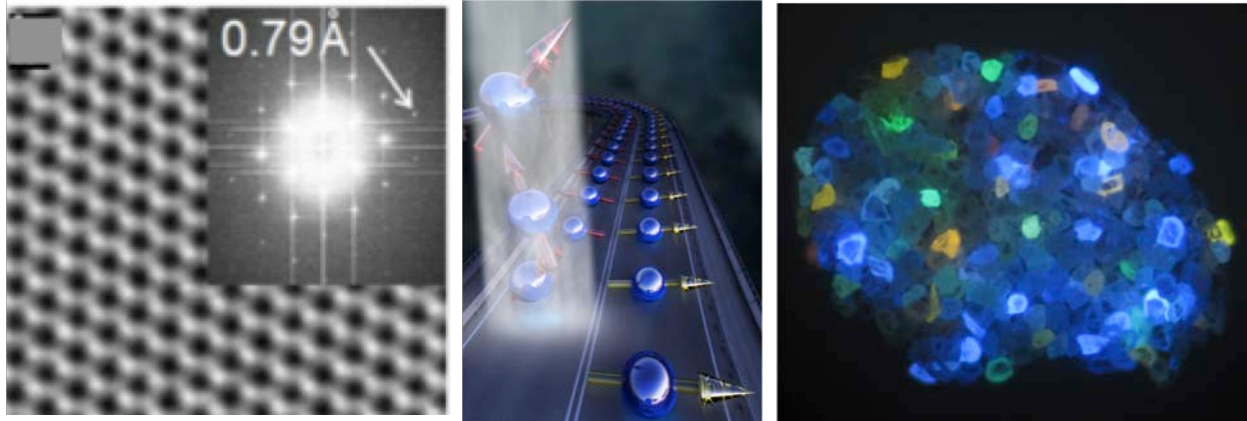


Fig. I.1 Quantum Materials: (left) High resolution TEM image of single atomic layer **graphene**, (middle) graphic - optical injection of spin qubits into a **topological insulator** edge state, (right) optically excited color centers in **diamond** microcrystals.

## I.2 Context Statement

### 1. Vision and Mission of our Center

**Vision** - Extraordinary new quantum materials enable atomic-scale electronics and photonics that transform signal processing and computation.

### Quantum Materials

In the past decade, quantum materials have been discovered that have extraordinary properties for signal processing and computation systems:

**Atomic Layer Materials** - Graphene (G), hexagonal boron nitride (BN), molybdenum disulfide ( $\text{MoS}_2$ ), and other transition metal dichalcogenide (TDMS) material layers, are only a single atom or molecule thick. Graphene has no energy gap; BN is an insulator, and  $\text{MoS}_2$  is semiconductor. These materials enable atomic-scale devices.

**Topological Insulators (TIs)** - Bismuth selenide ( $\text{Bi}_2\text{Se}_3$ ) and other topological insulators have conducting edge and surface states that topologically protect data by locking the direction of an electron's spin perpendicular to its momentum. TI materials can provide protected data channels.

**Nitrogen Vacancy (NV) Centers in Diamond** - The electron spin on an NV center can hold a qubit of information for  $> 1$  ms at room temperature, to act as a one-atom memory site. Data is optically programmed and read out. In addition, an NV center forms an ultrasensitive, high spatial resolution magnetometer, capable of imaging the field of a single electron spin at room temperature.

Quantum materials enable atomic-scale electronics and photonics that are based on their extraordinary properties. By integrating devices made from **Atomic Layer Materials** with data channels composed of **Topological Insulators** and memory sites from **NV Centers in Diamond**, our Center plans to build new types of **Quantum Electronic and Photonic Devices and Systems**.

## Mission

### Science & Technology

- Quantum materials allow electronics and photonics to pass beyond the limits of conventional semiconductors. Atomic-layer materials such as graphene enable ultrafast devices, topological insulators give error-free data channels, and nitrogen vacancy (NV) centers in diamond form atomic memory sites and sensors.

### Broader Impacts

- Our Center attracts young students to careers in Science, Technology, Engineering, and Mathematics (STEM).
- Our Center aims to achieve the gender and racial balance of our country.
- Our Center's Education and Public Outreach Programs engage young students and public audiences in the quest for new frontiers.
- Our Center's Knowledge Transfer Program commercializes research on quantum materials and devices into new products and technologies.

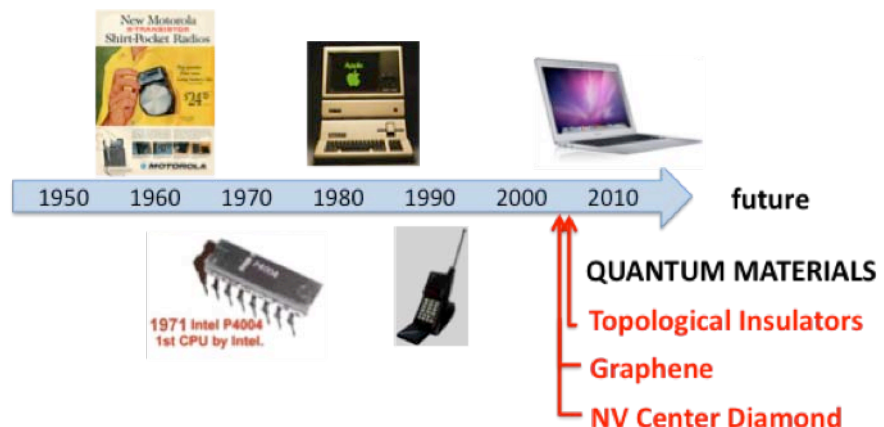
## Semiconductor Technology - Past and Future

CMOS technology has grown dramatically over the past fifty years, advancing from the creation of single silicon transistors in the 1950's, to portable radios in the 1960's, integrated circuits in the 1970's, desktop computers in the 1980's, cell phones in the 1990's, and to the portable computers we use today, as illustrated in Fig. 2. Quantum materials, discovered in the past decade, enable new devices and systems that change the rules. Quantum devices reach the atomic scale, they use single electron spins to store and transport information, and they create coherent qubits at room temperature.

CMOS technology has dominated electronics, because the scaling relations allowed the clock speed to increase as the device size decreased. The number of devices on a chip has increased, according to Moore's Law, to more than 1 billion. However, the clock speed stopped increasing a decade ago, and is now capped at a few GHz. According to the ITRS roadmap, this cap will be in place for the foreseeable future, even as the device size continues to decrease. Although CMOS technology will continue to dominate the electronics industry, it is time to look at new materials and new approaches for signal processing and computation.

Quantum materials are based on quanta of matter - atoms, electron charges, and spins - and quantum mechanics provides the basis for their operation. Quantum materials and devices open the way for truly atomic-scale electronics and photonics. Graphene and transition metal

Fig. 1.2 Timeline of silicon technology from the creation of silicon transistors to the present. Quantum materials, discovered in the last decade, offer pathways to atomic-scale electronics and photonics in the future.



dichalcogenide (TMDC) layers are outstanding conductors, even though they are just one atom or one molecule thick. And an NV center in diamond - composed of a single nitrogen atom and a single vacancy - can store a qubit of information at room temperature. In addition, topological insulators (TI) provide circulating edge states that transport spin without dissipation. These three classes of quantum materials promise atomic-scale devices, memory sites, and data channels for future electronics and photonics. They move the design space for electronics and photonics to interacting electrons and atoms, and away from the transport of classical particles.

## 2. Structure of our Center

Our Center brings together an outstanding group of researchers and educators. In this report we present the Structure of our Center, and we describe our Strategic Plan for the future.

**Section 3. Research Program** describes the long term Research Problems addressed by our Center: Quantum Materials by Design, Quantum Electronics and Photonics, Universal Quantum Interface, and Atomic-scale Networks .

**Section 4. Education and Public Outreach Program** describes our Center's Education Activities at the three Core Universities and the six College Network Schools, as well as our Public Outreach Program at the Museum of Science, Boston.

**Section 5. Knowledge Transfer** describes how our Center plans to commercialize science and generate new technologies by working with Harvard's Innovation Lab. Industrial and Innovation Partners help guide these activities.

**Section 6. Diversity and Human Resources.** Diversity is built into the structure of our Center with Howard as a core university, and through our College Network schools. Our Center actively recruit young students for careers in science and technology.

**Section 7. Management** describes the Administration of our Center and the processes by which money is allocated to its programs, and important decisions are made.

## 3. Research Program

Our Center's Investigators are shown in Fig. 3. The Center's research faculty members form a truly outstanding multidisciplinary group that includes leaders in the field of Quantum Materials. In Fig. 3, each investigator is near their initial research, although many investigators work on two or more types of quantum materials. The Research Program is divided roughly equally between Harvard University, Howard University and MIT. Research allocations and major decisions are made jointly by the Center's Executive Committee, as described in Section 7 below. Day-to-day matters is handled by the PIs and managers at each university: Gary Harris at Howard, Ray Ashoori at MIT, and Naomi Brave and Robert Westervelt at Harvard.

### 3a. Center Participants

To develop quantum devices and systems from quantum materials, it is essential to bring together experts with four types of expertise: 1) **Materials Growth**, 2) **Imaging and Material Probes**, 3) **Device Fabrication and Characterization**, and 4) **Theory of Quantum Materials, Devices and Systems**. The creation of new devices from quantum materials requires sequential steps: materials growth, characterization using imaging and material probes, device fabrication and testing, and theoretical understanding. For topological insulators, the cycle started with theoretical predictions of their unusual character.

Table I shows Center faculty researchers, grouped by their field of expertise - all three types of quantum materials are represented in each field.



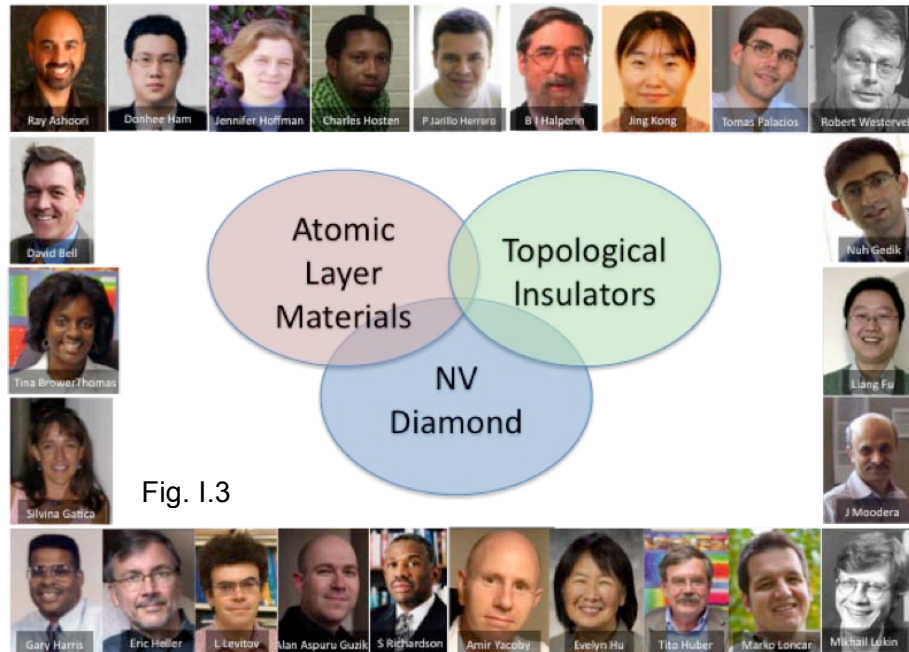


Fig. I.3

**Table I. Research Participants**

**Materials Growth**

<u>Tina Brower-Thomas</u> (Howard)	CVD growth of graphene
<u>Gary Harris</u> (Howard)	Growth of diamond and graphene
<u>Evelyn Hu</u> (Harvard)	CVD growth & processing of NV-center diamond
<u>Tito Huber</u> (Howard)	Growth and device fabrication of TI nanowires
<u>Jing Kong</u> (MIT)	CVD growth of graphene, BN, MoS <sub>2</sub>
<u>Jagadeesh Moodera</u> (MIT)	MBE growth of TI & TDMS materials

**Imaging and Probes**

<u>David Bell</u> (Harvard)	Electron microscopy of quantum materials
<u>Nuh Gedik</u> (MIT)	ARPES surface probes of TI materials
<u>Jennifer Hoffman</u> (Harvard)	Cooled STM of quantum materials
<u>Charles Hosten</u> (Howard)	Raman spectroscopy of quantum materials
<u>Robert Westervelt</u> (Harvard)	Cooled SPM imaging of electron motion

**Device Fabrication & Characterization**

<u>Raymond Ashoori</u> (MIT)	Graphene, TI, TDMS
<u>Donhee Ham</u> (Harvard)	Graphene, TDMS
<u>Pablo Jarillo-Herrero</u> (MIT)	Graphene, TI, TDMS
<u>Marco Loncar</u> (Harvard)	NV diamond, NV center qubits, diamond photonics
<u>Mikhail Lukin</u> (Harvard)	NV diamond, NV center qubits, qubit systems
<u>Tomas Palacios</u> (MIT)	Graphene, TDMS, integrated circuits
<u>Amir Yacoby</u> (Harvard)	Graphene, TDMS, TI, NV diamond

**Theory of Quantum Materials, Devices & Systems**

<u>Alan Aspuru-Guzik</u> (Harvard)	Correlated electron materials
<u>Liang Fu</u> (MIT)	Topological insulators
<u>Salvina Gatica</u> (Howard)	Graphene - chemical adsorption
<u>Bertrand I Halperin</u> (Harvard)	Correlated electron, spintronic and TI materials
<u>Eric Heller</u> (Harvard)	Electron transport in quantum devices
<u>Leonid Levitov</u> (MIT)	Graphene & hybrid materials
<u>Steven Richardson</u> (Howard)	Graphene analogs

### 3b. Shared Facilities for Materials Growth, Nanofabrication and Electron Microscopy

The Center's Universities have outstanding shared facilities for our Center's research: the Harvard Center for Nanoscale Systems (CNS) shown in Fig. I.4, the Howard Nanoscale Science and Engineering Facility (HNF), the MIT Microsystems Technology Laboratory (MTL), and the MIT Magnet Lab. In addition, Center collaborates with **Element Six Ltd** on diamond growth. Robert Westervelt is Director of CNS, and Gary Harris is Director of HNF. These shared facilities provide essential capabilities for our Center's research: 1) Growth of quantum materials: graphene, BN, TDMC materials, topological insulators, and NV-center diamond. via MBE at the MIT Magnet Lab (Jagadeesh Moodera), diamond growth at HNL (Gary Harris) and CNS (Evelyn Hu) and at Element Six, and CVD growth of graphene, BN and TDMC materials at MIT (Jing Kong). 2) Clean-room nanofabrication facilities for e-beam and optical lithography, focused ion beams (FIBs) and reactive ion etching (RIE) systems. 3) An excellent suite of electron microscopes at CNS managed by David Bell that include a Zeiss Libra-200 TEM, a new atomic-resolution JEOL ARM-200 STEM, and a Cameca Atom Probe that produces 3D tomographic images of material structure that identify individual atoms.

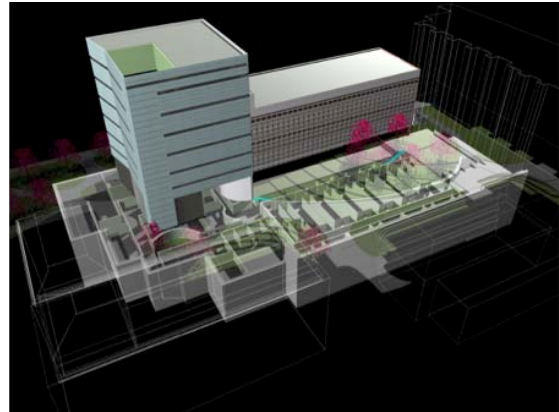


Fig. I.4 Harvard Center for Nanoscale Systems (CNS) - an underground 3-story building in the Laboratory for Integrated Science and Engineering (LISE).

### 3c. Science of Quantum Materials

The science of quantum materials is exciting, because it enables atomic-scale electronics and photonics. We give an overview of the scientific basis for these quantum devices and systems.

#### 3c1. Atomic Layer Materials

**Graphene** permits electrons to flow rapidly over long distances, even though sheets of the material are only one atom thick. As shown in Fig. I.5, the band structure of graphene is highly unusual, because the electrons and holes are massless and travel at a constant speed  $c = 1 \times 10^8$  cm/sec as if they were photons. This speed is larger than the carrier saturation velocity in III-V materials. The combination of high carrier speed, and short distances make graphene a natural material for high speed electronics.

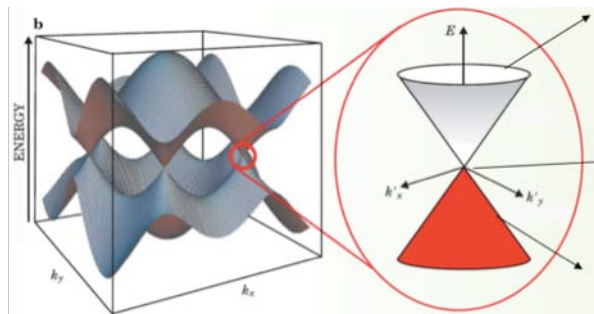


Fig. I.5 Graphene bandstructure.

In addition, electrons flow freely through graphene, enabling ballistic devices. This occurs because graphene has no energy gap - the electron and hole bands meet at a single point, called the Dirac point. The absence of an energy gap permits electrons to pass freely through a potential barrier - as the electron enters the barrier, it becomes a hole, and as it leaves, it becomes an electron again. This phenomenon - called Klein scattering - was predicted in the 1920's for relativistic particles, but had not been previously observed. The ability to pass freely through barriers allow electrons in graphene to have very long mean free paths  $\sim 1$  micron even though the material is only one atom thick.

**Hexagonal Boron Nitride** - Single atomic layer Insulating sheets are formed by hexagonal boron nitride (BN). The crystal structure of a BN atomic sheet is similar to graphene, except that the C atoms are alternatively replaced by a B or N atom. Insulating BN sheets are structurally matched to graphene, because B, C, and N are neighbors in the atomic table. By covering both faces of a graphene sheet with BN, one can make a high mobility graphene sheet that can lie on a substrate - the BN keeps adsorbed charges away from the conducting sheet.

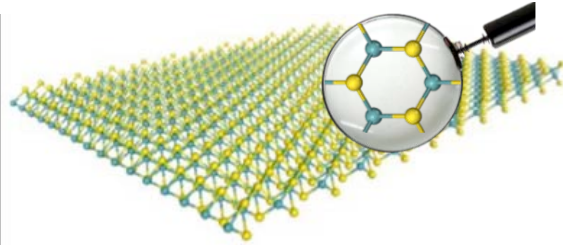


Fig. I.6 Schematic of MoS<sub>2</sub> monolayer.

**Transition Metal Dichalcogenide (TDMC) Materials** - TDMC materials such as MoS<sub>2</sub> form thin sheets that are one or more molecules thick (Fig. I.6). TDMC materials are often conventional semiconductors with useful bandgaps. For example, the gaps for MoSe<sub>2</sub>, WSe<sub>2</sub>, MoS<sub>2</sub> and WS<sub>2</sub> lie between 1 and 2 eV. As a result, TDMC materials can create switches with a large on/off ratio at room temperature. In addition, they can make optoelectronic detectors and emitters that can be used for applications, or to communicate optically with NV centers in diamond.

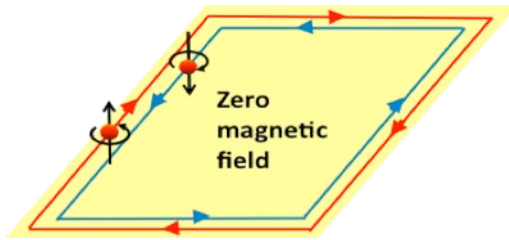


Fig. I.7 Circulating edge states of spin up (red) and spin down (blue) electrons in a 2D topological insulator.

### 3c2. Topological Insulators

Topological insulator (TI) materials - theoretically predicted (Kane and Mele PRL 2005, and Bernevig, et al. Science 2006) and experimentally verified (Konig et al. Science 2007) provide a topologically protected channel for data stored in spin states. A strong spin-orbit interaction polarizes electrons in zero applied magnetic field to form spin polarized edge states that circle the sample without dissipation (Fig. I.7), in the same way that edge states circle a 2D electron gas sample in the quantum Hall effect.

The spin direction is topologically locked perpendicular to the momentum, so that data stored on the spin is not lost, even in a collision with a non-magnetic scatterer. In a 3D TI material, the conducting states cover the surface, and they have a band structure like graphene with zero mass and no energy gap.

Topological insulators are in an relatively early state of development - the quality of currently known TI materials is being improved through careful growth to reduce bulk conduction, and new TI materials are being discovered - theoretically as well as experimentally.

### 3c3. Nitrogen Vacancy (NV) Center Diamond

Color centers in diamond are well known. However the recent discovery that an ionized nitrogen-vacancy center (NV-) can act as a memory site - storing a qubit of information for over 1 msec at room temperature - has created great excitement. In addition, the NV- center ion can act as a single-photon site to transfer the quantum information stored by the electron to a photon. Fig. I.8 illustrates the structure of an NV center in a diamond crystal. For the NV- ion, the spin 1 ground state is split between an  $m = 0$  state and degenerate  $m \pm 1$  states, separated by 2.9 GHz. The spin state can be written and read optically by shining green light onto the NV- center and observing the intensity of the emitted red light. In this way, the single atom memory site can be written and read.

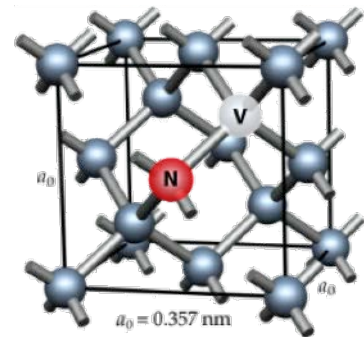


Fig. I.8 Schematic showing an NV center in a diamond crystal.



A single NV center is also a remarkably sensitive magnetosensor that can detect the magnetic field from a single electron spin at room temperature.

### 3d. Science & Technology of Quantum Materials, Devices and Systems

To guide our Center's programs toward important long-term objectives, our participants met to put together a Strategic Plan for the coming ten years. The initial All-Hands meeting with NSF staff was carried out on February 10-11, 2014, followed by an External Advisory Board meeting on March 10, 2014, and an additional All-Hands meeting on March 12, 2014.

The four Research Projects developed through this process will guide our Center's research program in the future toward its long-term goals. The focus of the original Research Areas on the three types of quantum materials will be redirected toward four Research Projects that emphasize important outcomes for our Center's research. Each Research Project uses all three types of Quantum Materials and involves a majority of our Center's participants.

#### LONG-TERM RESEARCH PROJECTS

Quantum Materials by Design

Quantum Electronics and Photonics

Universal Quantum Interface

Atomic-Scale Network

The strategic plan for each Research Project is summarized below, with mid-term goals and measures of progress.

#### 3d1. Quantum Materials by Design

Quantum materials are interesting and important, because the origins of their extreme properties were not previously known. Recent research has revealed that electrons pass freely over distances  $\sim 1$  micron through a single layer of carbon atoms in graphene, that the strong spin-orbit effect in topological insulators creates dissipation-free circulating edge state in zero applied magnetic field, and that an NV center can act as a single-atom memory site. For topological insulators, theory was in front, predicting phenomena that had never been observed.

A long-term goal of our Center is to create **Quantum Materials by Design**. As our understanding of the science advances, we can use this knowledge to guide the design of new quantum materials. Stacks of atomic layer materials, such as those shown in Fig. I.9, enable new types of quantum electronics and photonics, and new TDMC materials can be used to create low-power transistors and optoelectronic devices. The list of topological insulators is expanding rapidly to new compounds, with lower internal conduction and improved properties, guided by theoretical predictions. And advances in the materials science of NV centers in diamond will enable new types of devices and make it possible to expand the list of color centers used for applications in diamond and silicon carbide.

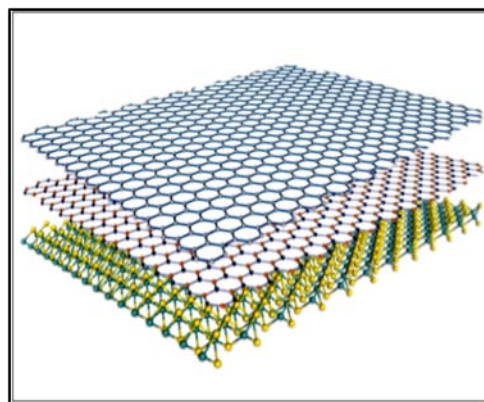


Fig. I.9 Schematic of a stack of atomic layers: (top to bottom) graphene, BN, TDMC layer.

## Growth and Transfer of Large-area Graphene Sheets

The highest quality graphene is currently obtained *via* sticky-tape exfoliation. For future applications, the growth of large areas of graphene will be essential. Jing Kong, Gary Harris and Tina Broder-Thomas are pursuing CVD growth of graphene, BN and TMDC materials. Figure I.10 shows a technique for CVD growth on a thin Cu substrate, which is later removed by a selective etch.

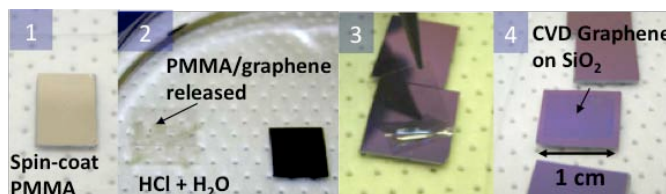


Fig. I.10 CVD growth of graphene on Cu and transfer to Si by selective etching (Kong).

Jing Kong also used a similar approach grow a two-layer G/BN stack. The measure of progress is the area of high-quality material. The challenge is to extend this approach to multiple layers of G or BN, and to layers of TMDC materials such as  $\text{MoS}_2$  or  $\text{MoSe}_2$  to grow atomic-layer stacks, like those in the next section.

## Atomic Layer Stacks

By stacking atomic or molecular layers of graphene, BN and TDMC on top of each other, hybrid layered materials can be created, which exhibit new types of quantum behavior opening the way for new devices. Boron nitride is a natural companion for graphene - BN provides thin insulating layers that passivate a graphene sheet. And BN/G/BN sandwiches provide a clear route to ballistic electron devices built on a substrate that avoid the difficulties associated with suspended graphene sheets.

An example of new quantum behavior is shown in Fig. I.11. Graphene transferred onto a BN substrate at an angle creates a Moire pattern between the G and BN lattices, which breaks the hexagonal symmetry and opens a bandgap up to 300K that is tunable by the tilt angle.

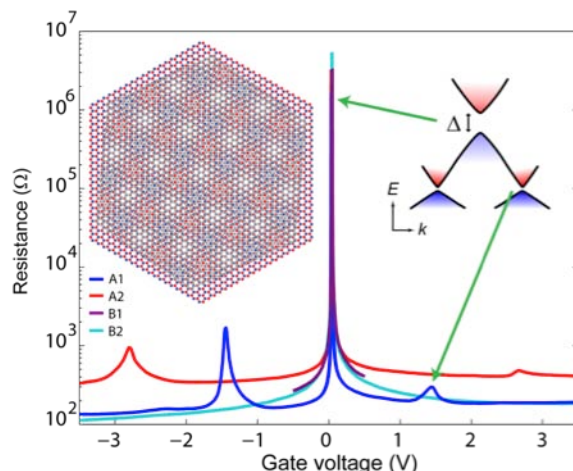


Fig. I.11 Resistance vs. gate voltage for a graphene transferred at an angle onto a BN substrate. The interaction opens up insulating states with bandgap up to 300K and mini-bands. (Hunt et al. Nature 2013)

Two layer BN/G/BN/G/BN sandwiches can create a tunneling transistor with graphene source and drain layers that are separated by a BN insulating layer, described in Quantum Devices below (Hunt et al. Nature 2013). Using this perpendicular tunneling approach, we plan to make spin transistors with tunneling transitions that conserve electron spin and pseudospin in two dimensions.

## Transition Metal Dichalcogenide (TMDC) Materials

Transition Metal Dichalcogenide (TMDC) materials can be exfoliated into sheets that are only a few molecular layers thick that act as semiconductors. Graphene, which has no bandgap, is difficult to use as a switch, because the off/on ratio is not sufficiently large. By contrast, TMDC materials can be grown with a wide range of bandgaps in the 0 to 3 eV range that are comparable to silicon and other conventional semiconductors, as indicated in Fig. I.12. Conventional transistors can be constructed from molecular-layer TMDC sheets, as well as optoelectronic emitters and detectors, and molecular layer TMDC devices can be used for a wide range of applications.

Our Center's research was initially focused on MoS<sub>2</sub> sheets: a single molecular sheet is a semiconductor with a direct gap, while a bilayer MoS<sub>2</sub> sheet has an indirect gap. We plan to broaden the range of electronic and optoelectronic applications by developing methods to grow additional TMDC materials, such as WSe<sub>2</sub> and to process them into devices.

### Topological Insulator Materials

Topological insulators (TIs) have fascinating physical properties. A challenge is to improve the material quality by reducing interior conduction so they can be used in devices. Our center focuses on TI growth, and the assembly of multilayer TI hybrids to transfer spin.

Using his MBE system (Fig. I.13) in the Bitter Magnet Lab, Moodera has grown a variety of topological insulator crystals and spintronic materials. Any of 15 different materials can be deposited in any order using 10 hearth electron gun sources, cooled 4K cells and an RF sputter source. Following growth, TI materials are separated by exfoliation into thin layers. A challenge is the growth of large area (~1 cm<sup>2</sup>) TI films with uniform and reliable properties.

At Howard, Tito Huber and Tina Brower-Thomas have grown BiSb (17% Sb) topological insulator nanowires. They plan to study their behavior of BiSb devices.

### Color Centers in Diamond

Nitrogen Vacancy (NV) centers in diamond have shown a spectacular success as single-atom memory sites, and as ultrasensitive magnetosensors. Our Center plans to develop techniques to position NV centers near the diamond surface to allow optical input/output to a given site with high spatial resolution. We are making NV-diamond photonic resonators, waveguides and nano-electromechanical systems (NEMS) to enable photonic applications, and plan to investigate additional color centers.

Our Center includes systems for the high-pressure growth of diamond and CVD diamond growth at the Howard Nanoscale Science and Engineering Facility (HNF) and a CVD growth system at Harvard. In addition, we have a strong partnership with Element Six, a leading firm in diamond growth, which foresees profitable near-term applications.

To grow diamond crystals with a layer of near-surface NV Centers, Element Six plans to delta-dope a thin layer of nitrogen into diamond < 10 nm below the surface during growth. The goal is to produce optically active NV centers for memory arrays, magnetosensors, and single-photon sources. Our Center also plans to ion implant N atoms into diamond near the surface, followed by annealing to remove unwanted damage. The challenge is to achieve functional near surface (<10 nm) NV centers.

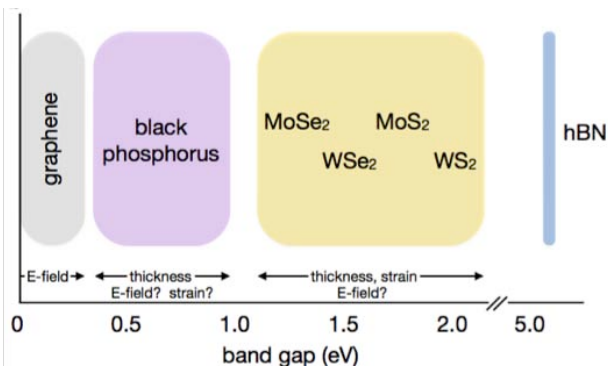


Fig. I.12 2D heterostructures with bandgaps in the 0 to 3 eV range.

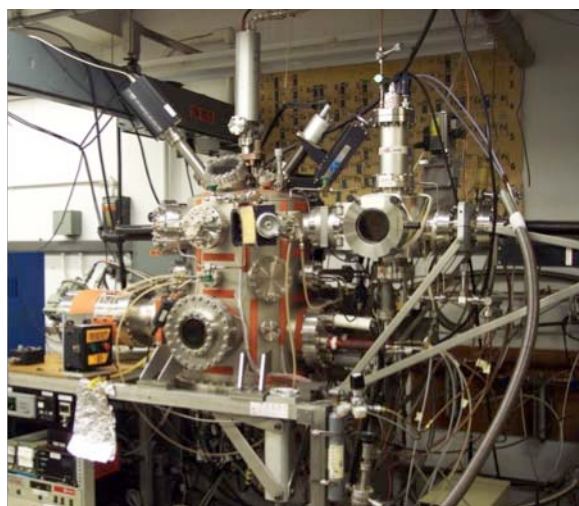


Fig. I.13 Molecular Beam Epitaxy system in Moodera's lab that grows topological insulator, TDMC and spintronic materials.



Nitrogen is a common impurity in diamond. A challenge for the future is to investigate the behavior of additional color centers, including boron, with the goal of obtaining long emission wavelength, optically detected magnetic resonance (ODMR) of color center spins, and bright sources of single photons.

### 3a2. Quantum Electronics & Photonics

Quantum materials are naturally suited to electronics and photonics with high speed and low power consumption. In graphene, the built-in speed of electrons and the short distances they must travel open the way for truly fast devices.

In addition, quantum materials have an extraordinary ability to manipulate and store spins. Topological insulator edge states protect spin states by linking the directions of the spin to the momentum, and graphene sheets can transmit spin states over long mean free paths. These unusual qualities are promising for low power electronics and electronics - manipulating a spin requires less energy than a charge.

Diamond NV centers open new routes for quantum memory and photonics. An NV center can store a bit of data for  $> 1$  msec at room temperature. A quantum bit of data can be transmitted from one place to another by using an NV center as a single-photon source that efficiently transfers the data from an electron spin onto a photon. Diamond's high index of refraction is well suited to photonic waveguides and resonators to implement these approaches.

#### **Ballistic Transport Devices**

The high speed and long mean free path of electrons in graphene enable the design ballistic transport devices, where the carriers pass freely between the sides of the structure. To make and test ballistic devices, imaging is important.

David Bell is using the high resolution Zeiss Libra 200 TEM in Harvard's Center for Nanoscale Systems to make atomic resolution images of graphene structures, such as the suspended graphene apertures shown in Fig. I.15. CNS is purchasing an atomic-resolution JEOL ARM200 STEM, which should prove to be a powerful tool for imaging atomic scale devices and structures. Imaging electron motion is also important, because the actual trajectory of an electron inside a ballistic device determines its properties. Westervelt is using a custom-made cooled scanning probe microscope (SPM) to image electron flow inside ballistic graphene devices. The charged SPM tip deflects electrons immediately below inside the graphene device, changing its conductance. By measuring the conductance as the tip is raster scanned above, the electron trajectories can be imaged.



Fig. I.14 Diamond growth facilities at Element Six Ltd, and in the Howard Nanoscale Science and Engineering Facility (HNF).

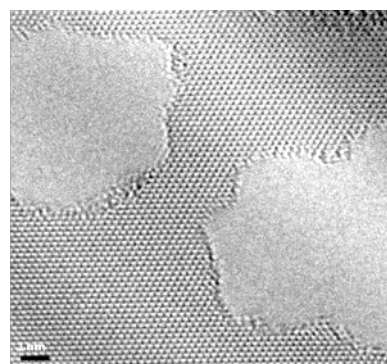


Fig. I.15 High-resolution TEM image of graphene (Bell).



## Quantum Devices

Vertical tunneling between graphene layers in BN/G/BN/G/BN stacks is an attractive approach. The vertical-tunneling transistor design shown in Fig. I.16 uses graphene layers as the source and drain. Theory and experiments show that the longitudinal momentum is conserved during the vertical tunneling process (Britnell et al. Science 2012). We plan to investigate the possibility that such structures will permit tunneling of spin and pseudospin states, creating a new class of transistors. Vertical transport favors speed, and the use of spin to carry data lowers the energy.

Transition Metal Dichalcogenide (TMDC) materials offer a wide range of opportunities for low-power electronics and photonics. Jing Kong and Tomas Palacios have developed integrated circuits based on bilayer MoS<sub>2</sub> devices, including an inverter, a NAND gate, a memory site and a ring oscillator (Wang et al. Nano Lett. 2012). A goal is to pursue this approach using other TMDC materials to develop functional circuit modules for conventional electronics and displays.

TMDC materials can also function as optical emitters and detectors with bandgaps up to 3 eV. An example is the WSe<sub>2</sub> photodiode shown in Fig. I.17 that emits at the wavelength 750 nm (Baughner et al. Nature Nano. 2014). A goal is to pursue the development of TMDC photoemitters and photodetectors for use in conventional optical displays and detector arrays.

An important long-term goal is to fabricate TMDC emitters and detectors on a diamond surface to provide optical I/O to near-surface NV centers used as memory elements. This diamond-based integrated electro-optic system is self-contained, and does not require external optics, greatly reducing the size and cost. An integrated TMDC / NV-diamond chip is an attractive approach for NV-center memory arrays for the Atomic-Scale Network Research Project below. In addition, the spacing of NV memory sites with TMCD

input/output devices can be subwavelength (< 500 nm), because the TMDC devices are in the near-field, adjacent to the NV centers.

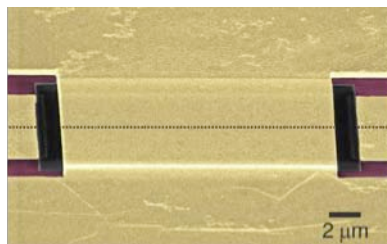


Fig. I.18 BN/G/BN waveguide used to measure the electron kinetic mass in graphene (Yoon et al. Nature Nano 2014).

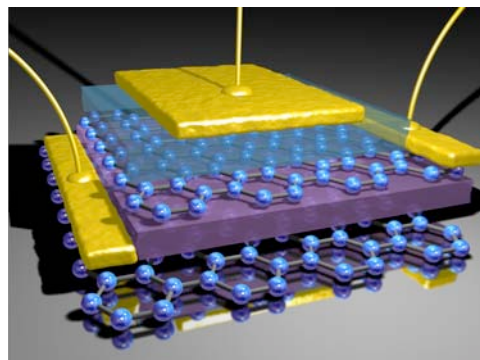


Fig. I.16 BN/G/BN/G/BN tunneling transistor design with a graphene source and drain. (Britnell et al. Science 2012).

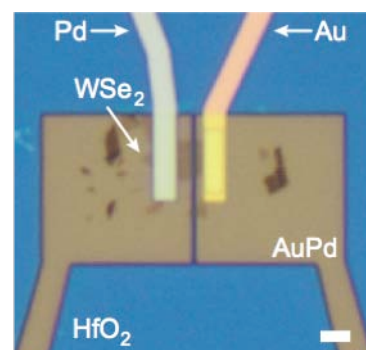


Fig. I.17 WSe<sub>2</sub> photodiode that emits at 750 nm wavelength (Baughner et al. Nature Nano 2014).

Graphene provides opportunities for ultra-high-speed plasmonic systems. As the frequency increases into the THz regime, the kinetic inductance associated with the electron mass takes over from the magnetic inductance, and one enters the plasmonic regime. Donhee Ham's group recently measured the kinetic inductance and the kinetic mass in graphene (Yoon et al Nature Nano 2014) using the BN/G/BN waveguide shown in Fig. I.18. This information will be used in the design of future photonic structures.

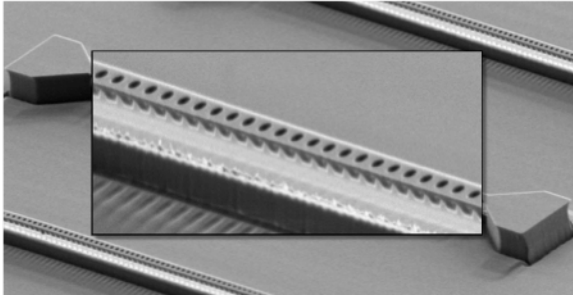


Fig. I.19 Diamond photonic resonator to couple NV centers (Loncar 2014).

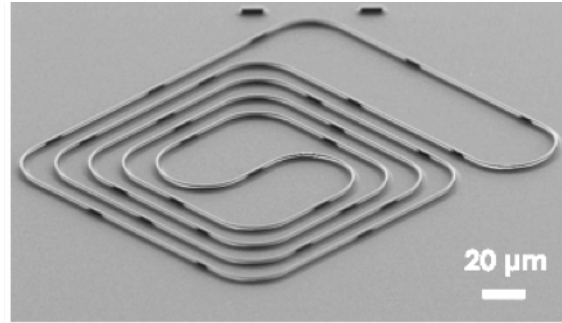


Fig. I.20 Diamond photonic waveguide above a diamond surface (Loncar 2014).

### Single Photon Sources and Diamond Photonics

Diamond nanowires permit a single NV center to act as a single photon source, for which only one photon is emitted at a time (Babinec et al. Nature Nano. 2010). Single-photon sources permit the transfer of a quantum bit of data stored on an NV center to a single outgoing photon. This capability allows an NV center to transfer the state of its stored bit to an external entity.

To efficiently couple an NV center to a photonic system, Loncar's group has created crystalline diamond photonic resonators, shown in Fig. I.19. NV-center resonators could serve as the basis for a diamond photonic network based on NV centers, or couple to external optics.

A photonic system can be created on the surface of a diamond crystal using diamond photonic waveguides. The waveguides are formed by a deep reactive-ion etch (RIE), which undercuts diamond channels, as shown in Fig. I.20. These waveguides can connect an NV center resonator to additional NV centers, to on-chip TMDC sources and detectors, or to an external optical system.

### 3a3. Universal Quantum Interface Research Project

Our Center plans to develop a Universal Quantum Interface to pass data from one quantum material to another - this function is essential to transmit signals through an integrated quantum system. Designing the interface is challenging, because the behavior of electrons differs from one material to another:

*Graphene* - massless electrons and holes that travel at a constant speed  $10^8$  cm/sec.

*MoS<sub>2</sub>* - electrons and holes with a finite mass and energy gap, like a semiconductor.

*Topological Insulators* - electronic surface states that lock spin to momentum.

*NV Centers in Diamond* - NV spin couples to photons, microwave fields, and strain.

Methods to inject and extract spin from Topological Insulator surface states must be developed to transport spin data through circulating edge states. Topological insulator spin-up and spin-down edge states normally circulate in opposite directions with no net current in zero applied magnetic field. Nuh Gedik used circularly polarized photons to inject a spin-polarized photocurrent

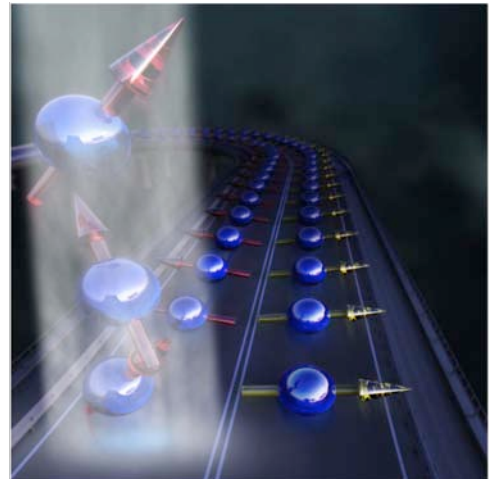


Fig. I.21. Circularly polarized photons inject a spin-polarized photocurrent in topological insulator surface states (McIver et al. Nature Nano 2012).

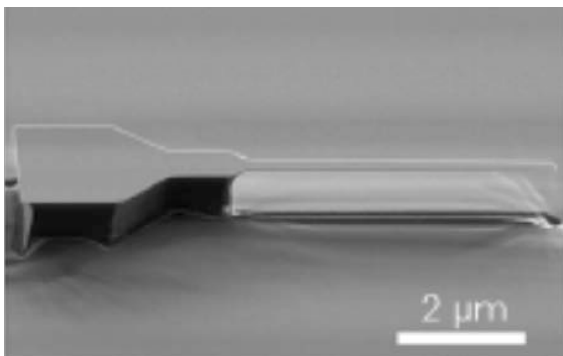


Fig. I.22 Diamond resonator to couple NV centers to strain (Burek et al. Nano Lett. 2013).

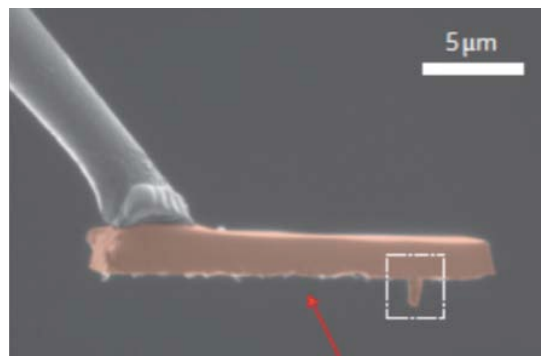


Fig. I.23 SEM image of an ultrasensitive scanning probe magnetometer with a single NV center in a diamond nanowire (Maletinsky et al. Nature Nano. 2012)

(McIver et al. Nature Nano 2012) as illustrated in Fig. I.21. A challenge is to implement functional TI data channels based on this approach.

TMDC optoelectronic sources and detectors fabricated on the diamond surface could provide I/O channels to NV centers located immediately below, as noted above (Fig. I.17). When on-chip device fabrication is realized, we plan to optically couple these devices to near-surface NV centers, using diamond nanowires, optical resonators, and photonics.

Mechanical strain provides an additional way to couple NV centers. By fabricating diamond nano-electromechanical resonators (Burek et al. Nano Lett. 2013) such as the cantilever made by Loncar's group (Fig. I.22), we plan to plan achieve efficient coupling of a single NV center to strain. Using strain provides a novel approach to coupling two NV centers inside an atomic network (see below). The ultimate targets are a resonator frequency  $f > 100$  MHz and quality factor  $Q > 100,000$ .

A single NV center in a diamond nanowire can serve as an ultra-sensitive magnetosensor with outstanding spatial resolution (Maletinsky et al. Nature Nano. 2012). Figure I.23 is a TEM image of an NV-center nanowire mounted on a scanning probe cantilever. The sensitivity at room temperature is sufficient to image a single electron spin on a diamond NV center below. We plan to use NV magnetosensor probes as a diagnostic tool to image currents or electron spin polarization in quantum electronic systems.

### 3a4. Atomic Scale Network Research Project

NV Centers in diamond have remarkable properties. An **Atomic Scale Network** integrates NV-center spins with TDMC electronics and optoelectronics on the diamond surface. An **NV-Center Memory Array** could be creating with optical I/O, first using external optics, then on-chip TMDC optical emitters and detectors. In the future, a **Diamond Computer Chip** could be created by integrating NV memory with surface TMDC electro-optic I/O and TMDC logic circuits. These projects are ambitious, and they demonstrate the promise of quantum electronics.

#### **NV Center Memory Array**

The first step toward an NV center memory array is to locate NV centers near the surface ( $<10$  nm) to allow optical I/O with high spatial resolution; an trial NV-center array is shown in Fig. I.24. Near-surface NV centers are being created via two approaches: nitrogen delta-doping during growth and nitrogen ion implantation followed by a high temperature annealing. We plan to balance the ion-implanting dose and array spacing, so that less than one NV occupies each site location, on average, to allow single NV centers to be addressed.

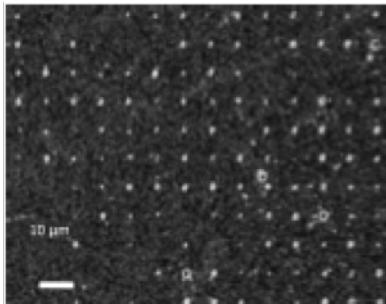


Fig. I.24 Ion-implanted array of N atoms in diamond.

To function as memory sites, the NV centers must be an NV-ion and have spectral stability to permit optical I/O. Both can be degraded by proximity to the surface and by crystal damage. A goal is to anneal structural damage following ion implantation to obtain a NV zero phonon optical linewidth < 100 MHz.

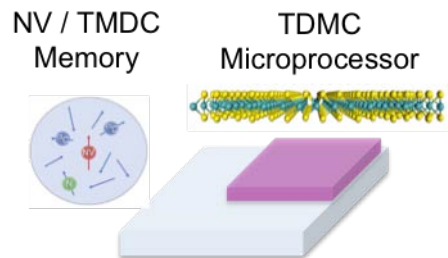


Fig. I.25 Concept for an integrated diamond computer chip with NV memory and on-chip TMDC optical I/O and logic.

Using on-chip TMDC electro-optical input/output channels, we plan to create an integrated NV memory chip without external optics. To move toward this goal, TMDC devices on diamond substrates are being developed in the Quantum Electronics, and Photonics Research Programs above. Optical coupling between the TMDC I/O devices and NV centers will be achieved by patterning the surface to produce diamond nanowires, resonators and photonic structures.

### ***Diamond Computer Chip***

For an advanced, long-term project, our Center plans to integrate a NV/TMDC memory array with on-surface TMDC logic to form a diamond computer chip (Fig. I.25). TMDC logic circuits on a silicon substrate have already been demonstrated, including a NAND gate, discussed above. The challenge is to demonstrate functional TMDC electro-optical devices and logic on diamond, and the long-term goal is to demonstrate the operation of an integrated diamond chip including both NV/TMDC memory and TMDC logic.

## **4. Education and Public Outreach Programs:**

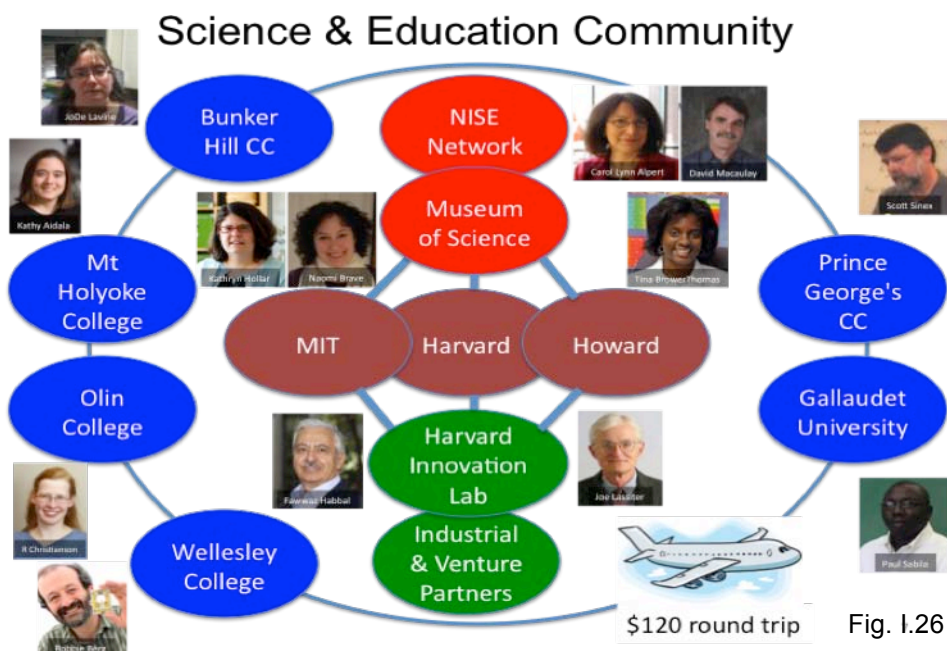
An essential goal of our Center is to attract, engage and retain young students to careers in Science and Technology. To do this, we formed the Science & Education Community shown in Fig. I.26. The Education Program at the Core Universities (Harvard, Howard, and MIT) is directed by Kathryn Hollar and Tina Brower-Thomas, with Public Outreach and Science Communication directed by co-PI Carol Lynn Alpert at the Museum of Science, Boston. Approaches to commercializing science are introduced to the students and postdocs at the Harvard Innovation Lab, directed by Joe Lassiter and Fawwaz Habbal. Our Center works with a strong group of Industrial Partners that includes IBM, Intel, and Microsoft Research, as well as Venture Capital Partners.

The College Network schools extend our the Science & Education program of our Center to a diverse group of students at community and 4-year colleges who would not normally gain experience in this area: The network includes Bunker Hill Community College, Mt Holyoke College, Olin College and Wellesley College in the Boston area, and Prince George's Community College and Gallaudet University in the Washington area. Mt Holyoke and Wellesley are women's colleges, and Gallaudet serves deaf and hard of hearing students. To bring these students into Center activities, we offer summer research internships, center-led seminars and courses, and academic-year independent-study projects.

### **4a. Academic Education Program Activities**

An important goal of our Center is to encourage young students to develop careers in Science and Technology through a range of activities described below.





Our Center's first summer internships began in June 2014. Each summer, College Network students work with university grad students and postdocs on research projects, taking advantage of our excellent shared facilities. After eight weeks, each student gives a presentation to the others, showing what they'd achieved. We plan to extend these student interactions during the academic year through independent-study projects and lab courses. Visits are easy and inexpensive, because the College Network schools are grouped together. A Washington-Boston travel fund is targeted at student exchange between center schools.

Harvard created a new course - Engineering Sciences 111 *Quantum Materials - from the Lab to the Classroom* - held in spring 2014. Each lecture presented highlights from our Center's research and education programs, and the lectures were WebEx'd to Howard, MIT and the College Network schools. In addition, Wellesley and Olin plan to create a joint Condensed Matter Physics course in the coming year.

During the 2013-2014 academic year, monthly Boston Area CarbON + Washington, (BACON+) meetings were held, to allow graduate students and postdocs to present their research to an audience of their peers. In addition, our Center students and postdocs hold Research Exchange talks to tell each other what they are doing - with no faculty present. These meetings provides a great way for the community to get to know each other - the talks are also WebEx'd to the other schools. In addition, Center students participated in the NanoDays event at the Museum of Science (see below) on April 5, 2014.



Fig. I.27 Gary Harris showing students the Quantum/Nano Express nanofabrication van from Howard University.

Howard University brings Nanotechnology to public schools and museums using the Quantum/Nano Express van that includes a complete nanofabrication and imaging lab shown in Fig. I.27. Howard drove the Quantum/Nano Express into the presentation area for the very popular USA Science & Engineering Festival held in Washington DC on April 25-27. Our Center held one of the BACON+ seminars there, as well an introduction to the Center by Bob Westervelt. In addition, Gary Harris presents the *Nanotalk* program on public radio, and Kathryn Aidala presents monthly *Science Cafe*'s for the public at Mt Holyoke University. Howard also provides a "Nano Boot Camp" to prepare public school teachers to teach nanotechnology in their classrooms.

On September 26-27, 2014 our Center will hold its first Annual Meeting. Each student or postdoc will give a 5-min talk about their research project, with posters and refreshments to follow. In addition, we plan to hold the first of an annual series of international Frontiers in Quantum Materials and Device workshops in Boston on December 4-5, 2014.

Naomi Brave, the Center's Managing Director, has developed a database program that longitudinally tracks the careers of Center students and postdocs, and relates their achievements to prior activities in Center events. We use the database to study the effectiveness of events such as Science Communication internships at the Museum, as well as to measure the benefit our Center to their careers. With their permission, the demographic data for participants is collected, to evaluate the effectiveness of programs for underrepresented groups.

An external evaluator measures the effectiveness our Center's Education and Public Outreach Programs. Students and postdocs provide written evaluations of four types of Center activities, including summer internships and the College Network student research experiences. In addition, the evaluator carries out interviews with individuals to obtain a more detailed view of the influence of the Center on education and in providing pathways to better careers. These interviews also evaluate the effectiveness of our Center's efforts to improve diversity in science and technology.

#### **4b Public Engagement and Science Communication - Museum of Science, Boston**

CIQM enjoys a unique partnership with the Museum of Science in Boston (MOS), building on twelve years of prior collaboration the Harvard-MIT-UCSB-MOS NSF Nanoscale Science and Engineering Center (NSEC). That partnership pursued a massive and ultimately successful experiment in public education about nanoscale science that produced 2,000 Museum stage presentations reaching 70,000 Museum visitors, and many more on the web, and dozens of guest researcher events. The partnership helped start the NSF Nanoscale Informal Science Education (NISE) Network, with Carol Lynn Alpert as founding co-PI and Robert Westervelt as Advisory Board chair. The NISE Network disseminates new educational subject matter and pedagogical techniques to hundreds of institutions across the country.

With CIQM, the Museum of Science team turns its focus to Quantum Materials:

**Aim 1:** Engaging broad audiences in the quest to explore and harness newly-discovered atomic-scale materials and phenomena.

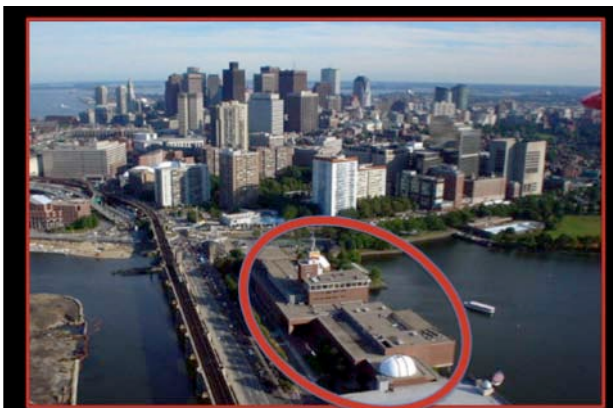


Fig I.28 Museum of Science, Boston

**Aim 2:** Work with CIQM students and postdocs to increase *their* capacity to share the motivation, process, and outcomes of their research.

**Aim 3:** Share knowledge about effective techniques with the broader STEM education field through publications and conference presentations.

**Aim 1** The MOS team is meeting with Center students, postdocs and faculty to brainstorm approaches to communicating, demonstrating, and visualizing their research. We are beginning with live museum presentations about atomic-scale electronics, guest researcher events, podcasts, hands-on demos, NanoDays activities, and video posted to YouTube.



Fig. I.29 Young students at the Museum.

On April 5, 2014 we introduced CIQM research at our **NanoDays** festival with Center graduate student running demos for young visitors, and a presentation by Bob Westervelt. In Year One, we are working with Gallaudet University to produce a sign-language interpretation of *The Amazing Nano Brothers Juggling Show*, and a bilingual version, and then in Year Two we will begin brainstorming for the new *Quantum Edition* of the production.

We are beginning to explore visualization sessions with David Macaulay, who has reached millions with illustrations in *The Way Things Work*, and CIQM faculty and students to visualize atomic-scale electronics. The graphics will be disseminated through the NISE Network, and they will be useful to College faculty in introducing these topics to their undergraduate students.

**Aim 2** The Museum team helps CIQM students increase *their* capacity to share the motivation, activities, and outcomes of their research with the public through our Sharing Science Workshop & Practicum, our Science Communication Internship program, and CIQM researchers speaking to Museum audiences. Year One has two Sharing Science workshops for students from the CIQM school. The first internship program will begin in January 2015.

**Aim 3** Activities in knowledge dissemination will pick up in Years Three to Five, when we have a body of work to share with others in the field.

## 5. Knowledge Transfer

An important mission for our Center is to develop effective pathways for intellectual exchange. Our Center's website <http://ciqm.harvard.edu> presents a full range of information about our Center and its activities. Educational materials are disseminated through the Nanoscale Informal Science Education (NISE) Network, and our YouTube channel (see above). In addition, we are forming productive partnerships with other institutions and industrial firms. We aim to instill a strong culture of commercialization and entrepreneurship in our participants, and to reduce the time-to-first-use for the Center technologies and ideas.

### Knowledge Transfer Goals

Goal I: CIQM students and postdocs serve as interns with industrial partners and, in turn, scientists from industrial and national laboratories spend time at the Center.

Goal II: Center participants build a portfolio of intellectual property around CIQM's materials, technologies, and devices.

Goal III: Our Center develops a culture of entrepreneurship and efficiently encourages the creation of start-up companies stemming from CIQM research.

Goal IV: CIQM achievements are disseminated into the broader R&D community through symposia and workshops, including government and industrial conferences.

Goal V: Additional funding for industry collaborations will be raised and government agencies will be stimulated to incorporate quantum materials and devices into their program areas.

These goals are furthered by establishing a strong group of industrial and innovation partners, organizing workshops focused on industry challenges, working closely with the offices of technology development at each university, developing patents, and establishing start-up companies related to the work of the Center.

The strategic plan for Knowledge Transfer, developed with full participation by all Center members, was presented at the External Advisory Board (EAB) meeting held in Cambridge, Massachusetts on March 10, 2014. The EAB members include Phaedon Avouris, IBM Fellow, and George Bourianoff, Intel Strategic Planning Group, as well other distinguished members with considerable experience managing NSF Centers and organizations. The EAB strongly endorsed the knowledge transfer strategic plan and recommended that an industrial session be included in the Annual Meeting, which has been incorporated into our plans.

Our Center has already recruited nineteen firms to be active partners (Table V). In the coming year, we will arrange summer internships for CIQM students and postocs, and exchange visits with scientists from industrial laboratories. In addition, our Center has recruited a team of experienced investors from the Innovation and Venture Capital communities to advise us on technology commercialization from CIQM discoveries as well as the licensing of our intellectual property on new quantum materials, quantum devices, and technology.

**Table V: Industrial and Innovation Partners**

Alcatel Lucent Bell Labs	Element Six	Intel	Qualcomm
Analog Devices	Epitaxial Tech	Khosla Ventures	Raytheon
Applied Materials	Graphenea	Matrix Partners	ST Microelectronics
BASF	Highland Partners	Microsoft Research	Texas Instruments
Blue Wave	IBM	North Bridge Venture	Vitesse



## 6. DIVERSITY AND HUMAN RESOURCES

### ***Diversity Goals and Objectives***

The diversity and human resources program at our Center has two major goals. Our first goal is for CIQM to become an exemplar and driver for institutional change in providing access to, and training for careers in quantum materials and STEM-related fields for women, individuals from under-represented groups, and military veterans. We aim to have the participants in our Center reflect the national demographics of these groups. For our Center, this specifically means working to achieve a more diverse and inclusive pool of potential graduate students and postdoctoral associates at Harvard and MIT, increasing the research infrastructure and opportunities for students at Howard, and expanding the career horizons of students in our College Network. The second goal for CIQM is to build a model for attracting and retaining deaf and hard-of-hearing students in the STEM fields. We will ultimately share this model as an adaptable template for our academic and industrial partners.

### ***Diversity Performances and Management Indicators***

Our Center balances the participation of women, underrepresented groups, and military veterans in our summer internship programs in partnership with our College Network. The College Network also serves as an invaluable source of STEM students for graduate study at Harvard, Howard and MIT. We will track participation during the lifetime of our Center.

### ***Human Resource Contributions***

CIQM participants from Howard and Harvard participated in the Third USA Science and Engineering Festival in Washington, DC on April 26-27, 2014. This event is America's largest STEM education event, and it provided a unique opportunity to introduce our Center to hundreds of potential STEM students in the greater Washington, DC area.

In June 2014, our Center began its first Summer Internship Program for Undergraduates at Harvard, Howard, MIT, and the Museum of Science. The focus was to provide research experiences for a diverse group of College Network students.

Our Center supported the following women in 2013-2014 through our CIQM Postdoctoral Fellowship for Women and Minorities Program: Birgit Hausmann ([Marko Loncar](#)), Nathalie de Leon ([Mikhail Lukin](#)), Lan Luan ([Amir Yacoby](#)), and Lili Yu ([Tomas Palacios](#)).

### ***Diversity Plans***

- Provide training of laboratory best practices for CIQM participants for collaborations with deaf and hard of hearing students.
- Recruit faculty and students to present at the annual Society for Advancement of Chicanos and Native Americans in Science and National Society of Black Engineers.
- Create research collaborations for deaf and hard-of-hearing students at Harvard, Howard, and MIT.
- Provide opportunities for College Network students to engage with K-12 students and the public at the Museum of Science.



Fig. I.30 CIQM Kick-Off at Howard University.

## 7. Management

Our Center consists of forty faculty and staff at ten institutions, with important collaborations at industrial firms, international institutions, and the national laboratories. Our Center offers dynamic educational programs through the College Network for students and teachers at all academic levels, and it pursues unique opportunities to bring this research to the public through innovative programs with the Museum of Science, Boston.

Research allocations and other major decisions are made by the Executive Committee. The PI and Director is Robert Westervelt at Harvard, who works with co-PI Gary Harris at Howard University, co-PI Raymond Ashoori at MIT, and co-PI Carol Lynn Alpert at the Museum of Science, Boston. Research on the three groups of quantum materials is coordinated by: Atomic Layer Materials (Pablo Jarillo-Herrero), Topological Insulators (Nuh Gedik), and NV Center Diamond (Marko Loncar). Knowledge Transfer and Industrial Partnerships are led by Tomas Palacios. Advice on Center management is provided by Evelyn Hu. In addition, the Executive Committee includes CIQM senior staff: Managing Director Naomi Brave, Gordon McKay Laboratory Director Robert Graham, Education Directors Kathryn Hollar for Harvard and MIT, and Tina Brower-Thomas for Howard University.

Research Allocations are decided each year, based on reported progress in the previous year, and a proposal for the coming year. Collaboration with at least one Center faculty member is required, and collaboration with investigators outside the Center is encouraged. The allocation process is open to faculty members who are not currently part of the Center, and current participants are let go if they do not carry out collaborative research, or veer away from the Center's goals. In addition, innovative proposals are approved during the year as Seed Projects. The CIQM Executive Committee also considers capital equipment expenditures, evaluates staff appointments, and has an active role in the allocation and budgeting process.

The External Advisory Board evaluates the Center's programs and performance, and provides strategic advice. The members are Ilesanmi Adesida (University of Illinois at Urbana Champaign), Phaeton Avouris (IBM), David Awschalom (University of Chicago), George Bourianoff (Intel), Robert Chang (Northwestern University), Fiona Goodchild (UC Santa Barbara), Jorg Kotthaus (Ludwig Maximilian University), Monica Olvera de la Cruz (Northwestern University), and Andy Vidan (MIT Lincoln Laboratory).

The Internal Advisory Board provides advice on Center decisions during the fiscal year. The members are Federico Capasso (Harvard), Mildred Dresselhaus (MIT), Fawwaz Habbal (Harvard), Patrick Lee (MIT), and James Mitchell (Howard University).