Robert A. Wolkow Scientific Biography March 2019

Wolkow has had a leading role in discovering, altering and deploying atom scale properties of silicon. His years of fundamental advances have laid a broad foundation for practical applications. With his spin-off companies, he is initiating commercialization.

Aspects of his work:

- Decades of consistently cutting edge studies of atom-scale properties of silicon surfaces, primarily with scanning tunneling and atomic force microscopies, complimented by extensive instrument development and theoretical modeling
- Unique, exacting studies of the dynamics, structures and properties of single molecules and ensembles attached to silicon–
- Led the new area of exploration involving the Si dangling bond as an atomic quantum dot that enables diversely capable ensembles
- Truly transformative advances in fabrication tools and methods for atomic silicon ensembles
- Recognized many relative advantages of atomic Si circuitry:
    - dots are identical. Also spacing and therefore interaction among dots is identical because rigidly governed by the crystalline Si lattice
    - connections/electrodes among active elements are free of the traditional interfaces responsible for charge traps – a huge differentiator
    - Si atomic circuitry has states in the bulk bandgap, preventing short circuiting by the bulk
    - ultimate small Q Dots enable extreme close spacing, resulting in extremely strong interactions among dots, yielding:
        - noise immunity
        - ability to work at room temp for classical applications
        - relaxed cryogenic requirements in the quantum applications space

    - All the diverse passive and active components required to create circuitry are – amazingly - formed of one common building block, the atomic Si Q dot, and printed in one pass.
    - No implanting, masks, alignment, resists, vias – no multilayers
    - All Si and merged with CMOS. Atom circuitry will be an on-chip enhancement to circuitry that is 95% CMOS. The atom components will be limited to ~10,000 atoms initially – a manufacturable number. Projecting ~1 million chips per year production is within reach

- Key elements for an ultra low power yet extremely fast binary atomic silicon logic proven
- “Killer Apps” – viable, valuable, first applications and strategic commercial partners identified.
    - Demonstration of an atomic electronic machine that is a simulator of Ising type system and therefore can be configured as a Gibb’s sampler allowing a new paradigm for un-supervised neural network training. In partnership with 1Qbit.
    - With Samsung ultra fast and low power flash analog to digital converts are being developed to enable a new hybrid analog and digital approach to computing that promises huge energy savings.
- 2 businesses started (advanced tools), 2 more starting – based on atom circuitry

This document has 2 parts, as follows:

PART 1

- early work/1997 up to about 2005
- The “Chemical Physics” phase: many exacting studies of molecules on silicon

PART 2

- 2005 to 2019
- stopped working on molecules, started building artificial molecules and circuitry elements with Silicon atoms
- Discovered many insights into character of Si dangling bonds
- single atom tip, “world’s sharpest object”
- patented atomistic quantum dot
- proved potentially revolutionary circuitry concepts
- At this time when it has become universally accepted that silicon technology has reached a point of maturation, he says no, CMOS is mature, but there is tremendous growth yet to come in silicon technology
- Cutting edge research and student training continues – but large effort in commercialization also

PART 1

After completing his PhD in Toronto Wolkow became a postdoc at IBM Yorktown Heights, NY in 1987. Starting with an empty room, he quickly established a scanning tunneling microscope (STM) lab and soon after became the first person to gain an atom-resolved view of a chemical reaction. He and his supervisor Phaedon Avouris explained that upon reaction, the elimination of Si surfaces states and the concomitant formation of new electronic states outside the energy window probed by the STM, accounted for the dark appearance of adsorbates in STM topographs. Large observed differences in reactivity among seemingly identical surface sites was correlated with measured inequivalent local state density of atoms in the unit cell. The utility of these insights for understanding molecular images endures to this day. Their Physical Review Letter **60**, 1049 (1988) and Phys. Rev. B **39**, (1989) of the study are highly cited (422 and 356 times) and the figures from those works have appeared in specialist's and introductory texts as well as in many lecture notes. Avouris and Wolkow (after leaving IBM) shared the T.J. Watson IBM Outstanding Achievement Award in 1989.

The above work caught the attention of AT&T Bell Labs, leading in 1988 to an invitation to visit and then an on-the-spot job offer. As a member of the technical staff at AT&T Bell Labs at Murray Hill, he decided to create the first tunable temperature, cryogenic STM – a task many at that time recognized as the most crucial next step for the field, but one that seemed impossible due to extreme thermal drift issues. It took near 3 years, but he did it. The most notable early application of this new instrument led to his 1992 PRL (cited 808 times) that settled a controversy unresolved since 1958 - regarding the remarkable structural dynamics of the Si(100) surface (the surface virtually all circuits are built on). Wolkow's results confirmed that the silicon dimers on that surface act as bistable teeter-totters, collectively exhibiting an order-disorder transition – in close analogy to an antiferromagnet. Innumerable studies have been informed by and built upon his result, and, that surface and his ground breaking results remain highly topical today – both the areas of classical atomic circuitry and in Si-based quantum computing.

In 1993 Wolkow was recruited by the NRC in Ottawa to form the Molecular Scale Devices group. He focussed on chemical physics problems with a particular interest in the then baffling problems in molecule-silicon surface bonding. His 5 publications on the prototypical case of benzene on Si(100) have collectively received 605 citations. He calculated properties of diverse adsorbed structural candidates, he simulated images and calculated and measured vibrational spectroscopy too. One studied species undergoes a transformation in time to a more strongly bonded entity - he both measured and calculated the barrier controlling that process - typifying the depth of his studies.

His tour de force work to isolate and characterize weakly bound molecular precursors to strong covalent bonding – predicted in the 1930s by Langmuir but never previously observed – provided a seminal insight into that ubiquitous process. The precursor state was captured at low temperature, and the kinetics of its decay to the strongly bonded state were measured. The well depths of the physical and covalent bonded states as well as the height of the barrier separating them were determined. That barrier was recognized as the cost of a configuration change of the molecule, a re-hybridization to enable strong bonding. Science 279, 542 (1998), cited 135 times. This work is covered in several texts also.

Soon after, using STM and quantum mechanical calculations Wolkow showed for the first time the ability to recognize individual chiral molecules on a Si surface while also explaining how racemization during the stepwise attachment reaction could occur [Nature 392, 909 (1998) cited 268 times] and [J.Am.Chem.Soc.

122, 3548 (2000) cited 84 times]. His review "Controlled Molecular Adsorption on Silicon: Laying a Foundation for Molecular Devices" Ann.Rev.Phy.Chem. **50**, 413 (1999) has been cited 708 times.

In Nature **406**, 48 (2000) cited 642 times, Wolkow showed the first method to create covalently bonded, self-assembling, ordered, multi-molecule nano-structures on Si. The work was later greatly extended by others. This is an amazing process: one needs only "point" at a desired site, and then leak reactant molecules into the vacuum chamber to see ordered structures form in a predetermined way. It is like polymerization, but different because the molecules do not bond together to form a chain, instead each molecule is firmly bonded to the Si surface. Wolkow has described these lines as like ordered liquids. The initiation site was created by tip assisted removal of one H atom from a H-terminated silicon surface resulting in in a single silicon dangling bond. Wolkow knew from his previous studies that most organic molecules require not one, but two adjacent attachment sites in order to stably bond. By providing only one surface attachment site, he knew he would create a weakly bonded, transient species. For example, an alkene can open its pi bond (retaining its sigma bond) to create two attachment points. When one carbon joins with the silicon dangling bond to form a C-Si covalent bond, one 3-coordinate, very reactive carbon radical remains on the molecule. Bound by only ½ an eV or less, such a species detaches to reform the double bond in a microsecond or less at room temperature. But cases were designed where the carbon radical could extract a hydrogen atom from an adjacent surface site, thereby creating a very stable, surface bound molecular species, and, a new adjacent silicon dangling bond where another molecule could attach. Repetition of the process allowed lines of molecules to form. The straight, equally space molecular lines "borrowed", in a sense, the crystalline order of the substrate.

Using this new approach, rational design of otherwise impossible to obtain highly local tuning of the surface potential of the silicon substrate was demonstrated by forming multiple parallel lines of molecules containing a very large built-in dipole moment. Such abrupt potential gradients could not be formed by any conceivable electrodes. PRL 101, 106801 (2008)

It is remarkable that the human-scale action of turning a valve allowed more such molecules to be added at will. Growth could be halted by closing the valve while the bottle of molecules was changed, then, upon reopening the leak valve, molecules of a different kind could be added, creating beautiful, entirely unique, 1-dimensional molecular heterostructures. The rich electronic properties of these species and their sharply defined molecular interfaces were explored in joint studies with theorists George Kirczenow in Phys. Rev. B 72, 245306 (2005) and with Hong Guo, JACS. 131, 11019 (2009) and Nano Lett. **17**, 322 (2016). Many further insights were gained - like how to make a robust diode that is lateral, not normal to the surface, for example.

Multiple other avenues for the self-directed line growth process were explored. Lines of ferrocene molecules, each carrying one Fe atom, were likewise grown [Nano Letters 2, 807 (2002)]. Lines of "radical clock" molecules were used to learn about stepwise rates of the growth process by watching which of two possible branching outcomes occurred [Nano letters 4, 357 (2004)]. Methods to change the direction of line growth were also explored [Nano letters **4**, 979 (2004)] and [J. Phys. Chem. A **111,** 12257 (2007)].

Wolkow's original theoretical descriptions of the line growth process accounted for the inability of very small alkenes to grow lines, and the ease of line growth when an alkene was coupled to a benzene ring. Calculation showed that the ring lends tremendous stabilization to the radical intermediate species, giving time for H abstraction from the surface to occur. Surprisingly, simple 1-alkene's with an aliphatic tail were shown to grow lines despite missing the stabilization of the aromatic ring - a surprising result initially. The

key in that case was physical adsorption of the molecule tail to the Si-H surface, leading again to a sufficiently long lived radical species - but for a entirely different reason J.Phys.Chem. B **110**, 2159 (2006). Studies done with theorist Gino DiLabio led to improved computational methods and understanding of the role of dispersion interactions in such systems.

While the impact of much of "molecular electronics" research is limited because numerous variables were undefined, this sampling of Wolkow's molecule-silicon work, by contrast, shows well defined studies that will serve as reliable reference points to learn from and build upon. Work of this period led to the Noranda award for physical chemistry and the Royal Society of Canada Rutherford medal for physics.

During this period Wolkow became both a NRC Principal Research Officer and a Fellow of the Royal Society of Canada, in both cases among the youngest ever to be so recognized. Around that time, he also chaired the International STM conference, in Vancouver, a meeting with about 650 participants. Later he co-chaired the Gordon Research Conference on Nanoscale Fabrication. He also was elected "Member at Large" of the American Vacuum Society. In 2002 Wolkow co-authored an influential white paper that was the beginning of Canada's National Institute for Nanotechnology (NINT). In 2003 he was recruited by the University of Alberta in Edmonton Alberta. He was awarded the iCORE Chair in Nanoscale Information and Communications Technology and became simultaneously Principal Research Officer and Molecular Scale Devices Program Leader at the new National Institute for Nanotechnology he helped initiate.

PART 2 Dangling Bond Patterning *(Stop placing molecules. Make molecules in place.)*

In "Field regulation of single-molecule conductivity by a charged surface atom", Nature **435**, 658 (2005), 338 citations, Wolkow and co-workers introduced a powerful new concept: The Si dangling bond as an active electronic entity. In this early study they showed a neutral dangling bond had no effect on adjacent molecules whereas a negatively charged dangling bond caused a Stark shift and a gating of current through the molecule. This finding underpinned a subsequent series of remarkable papers (and patents) in which he has shown how to control diverse conduction channels with extremely high gating efficiency – hugely more desirable than popular break-junction experiments of the time where molecule configuration was entirely unknown and gating efficiency was extremely poor – requiring unattractive high voltage to compensate.

Enough bottled molecules

That 2005 paper marked a turning point in Wolkow's work. He turned away from carefully positioning and characterizing molecules on silicon. He felt he could make more progress if he could learn to exactingly define dangling bond ensembles of diverse function. In a sense, he planned to make molecules, along with ideal connections, rather than attempt to position molecules from a bottle. Moreover, he had shown in a series of highly detailed studies, experimental and theoretical, that many attractive molecular functional units would soon degrade upon carrying a current - Surf. Sci. **457**, L425 (2000) cited 77, Faraday discussions **117**, 213 (2000) cited 38, Phys. Rev. Lett. **85**, 5372 (2000) cited 122, and Nano Lett. **6**, 390 (2006) cited 74 times.

By the new approach, it would become possible to both exactingly define molecule-like entities, and, perfectly define connections to and among those. As always for Wolkow, experiment and theory were an inseparable pair of activities. His single minded, unique goal took about 15 years to accomplish, but through a series of papers, and patents, he has done it.

Atomic Patterns of Incomparable Stability and Utility

Whether using directed nano-patterning or using spontaneous self-assembly, most of Wolkow's peers are studying adsorbates on metal substrates. While it is commonly rationalized that one can establish methods of assembly on a convenient metal surface, and later worry about transferring the work to an electronically useful surface, Wolkow regards such approaches as non-starters. Metal substrates short-out any potentially useful properties of nano-assemblies formed. And efforts to transfer an adsorbate assembly process to another substrate is essentially starting over - little built-up knowledge of assembly or of assembly properties will transfer - changing substrates is starting over. The situation is improved by adding an intervening salt layer, but that results in week bonds to the substrate and unstable, impractical assemblies.

Wolkow's gap state derived electronic structures are disconnected from bulk conduction channels yet benefitting from the regular lattice the Si substrate imposes on ensemble geometries.

Another feature, and debilitating problem, common to most all other nano-fabrication efforts aiming for future device is temperature instability. Virtually all atom-scale scanned-probe manipulation processes being studied result in structures that cannot survive above extreme cryogenic conditions. It is not possible to use or even transport such structures at 300 K. Wolkow's structures are entirely stable to 500 K. The simple wafer-bonding encapsulation he has planned will make those environmentally stable also.

A third outstanding aspect of his approach is macro to atom-scale connections. On the input side, his spin-off company QSi has developed lithography whereby atom-scale extensions of normal lithographic features engage (by electric field) with his atomic circuit elements, allowing the binary state of atomic elements to be dynamically controlled through simple low voltage bias controls. To return information from the atom-scale he has created the first-ever perfectly identical, SETs (single electron transistors) that will transduce binary state encoded as electron position to a current that is readily accessible to conventional transistor based CMOS circuitry. His atom defined SETs are all the same. All other SETs are made using lithographic processes with uncertainties larger than the designed dimensions resulting in extreme device variability. While he has his sights on much more complex circuitry, these SETs alone appear to be important detectors and circuit elements. In addition to being reproducible, his devices do away with all the electrodes and interfaces that form charge traps that plague other quantum dot devices. His Coulomb blockade energy is enormous, of order 100 meV, allowing room temperature operation.

Perfecting Patterning

Bob always acknowledges that his patterning approach is an extension of an idea due to Tucker and Lyding. Over 2 decades ago they showed the remarkable ability to desorb lines and patches of H atoms from hydrogen terminated silicon. It was reasonably presumed then that adjacent silicon dangling bonds would exhibit some significant degree of electrical connectivity, which has recently been proven to be true

However, despite many efforts, including the commercial effort by Zyvex Labs to exactly define dangling bond arrays, little progress toward perfecting patterning was made. Zyvex has not yet succeeded after a decade long effort to make exactly fabricated objects - with a precisely known number and geometry of atoms, that could serve, for example, as nano-scale length standards.

Some time ago, Wolkow showed that carefully reproduced pulses of current between a scanned probe and a surface created a distribution of desorption results, Surface Science **600**, L199 (2006) cited 33 times. It was clear that tip condition, that is, atomic structure of the tip apex was varying and causing uncertainties.

Around the same time, Wolkow had come up with an striking method for making reproducible single atom tungsten tips. In "Tungsten nanotip fabrication by spatially controlled field-assisted reaction with nitrogen", Journal of Chemical Physics 124, 204716 (2006), cited 127 times, Wolkow came up with a new approach to scan probe fabrication that resulted in identical single atom tips.

While using a home-made Field Ion microscope (FIM) for imaging the atomic structure of an electrochemically etched tip, it was discovered that ordinary nitrogen gas, N_2, would dissociatively adsorb on the tungsten surface to create atomic asperities that become "lightning rods", subject to field evaporation under high electric field imaging conditions within the FIM. Etching proceeds in this way –

exclusively at the shank of the tip. The field could be adjusted so that nitrogen approaching the tip apex was readily field ionized and propelled away before it reached the surface (much as the helium imaging gas is ionized and pushed away as He^+). But, at the same field that prevents nitrogen reaching the apex, regions of lower curvature and therefore lower field become chemically attacked by nitrogen, leading to etching all around the apex. An atom-by-atom movie of the process must be seen. Go to https://www.robertwolkow.com/movies, click "Making a single Atom Tip".

Many school children know about this tip because it is in the Guinness book of world records under "Sharpest object man-made". It is covered by 2 patents. The tip features in two papers describing a holographic electron microscope Wolkow's team built. "Low-energy electron point projection microscopy of suspended graphene, the ultimate 'microscope slide', New J.Phys. 13, 063011 (2011) and, "Nanoscale structuring of tungsten tip yields most coherent electron point-source", New J. Phys. 15, 073038 (2013). Bruker of Germany studied those papers. Now, Wolkow's company QSi is licensing the technology to Bruker and he is creating another company that will manufacture the atom sharp tips and sell them under contract to Bruker. The new Bruker instrument will be a powerful new instrument that can rapidly determine single molecule structures - crucially, the molecules do not have to form ordered crystals as required for practical x-ray diffraction based structure determination. This could turn out to be a tool of great scientific impact.

Atomic Editing

Returning to silicon atom studies as enabled by his new tip:

Getting a tip to perform well in a scanned probe microscope has generally been more craft than science. But now, by attaching a home-made Field Ion Microscope to each of his scanned probe instruments which allows near perfect tips to be made, Wolkow has made excellent scanned probe performance a virtual certainty, and, his tips have in turn led to greatly improved H-removal characteristics. However, several percent error rates – removal of an H from the wrong position - remained. Perfect patterning had to await another advance, one that allowed replacement of H atoms to deterministically removed undesired dangling bonds.

While every researcher working on H-Si observed occasional uncontrolled capping of silicon dangling bonds no one had discovered a reliable process for dangling bond capping with H. Wolkow's team recently did so. A combination of known FIM-based tip fabrication procedures as described above and loading of the tip with H atoms was found. A suitable H loaded tip holds the H atom at its apex, as evidenced by extra large corrugations in topographic scans. Proper mechanical alignment reliably transfers the H atom from tip to Si dangling bond to form a robust Si-H species. This is described in "Atomic white-out: Enabling atomic circuitry through mechanically induced bonding of single hydrogen atoms to a silicon surface", ACS nano 11, 8636 (2017). Multiple improvements in the process were soon made and described in "Lithography for robust and editable atomic-scale silicon devices and memories", Nature communications 9, 2778 (2018). There, all the letters of the alphabet were written in ASCII code. The super Mario theme music was written as well. This was the highest information density ever written. And, unlike data written with previous atom patterning schemes which all would evaporate well below -200 C, these patterns are stable to +200 C. Patents have been filed.

“Impossible” problems solved with Machine Learning

One further crucial step occurred to transform the prospects for atom scale fabrication of robust and useful atom-defined ensembles. Even with the unique and effective tips now routinely prepared by the group, occasional inevitable deleterious tip changes occurred during scanning that required laborious, time consuming reconditioning of the tip. It was known that very gentle application of a field between tip and sample could drift aberrant tip atoms back into a desired state. But application of that tuning process required a delicate hand and many tries before success. Last year, “Autonomous Scanning Probe Microscopy in Situ Tip Conditioning through Machine Learning”, ACS nano 12, 5185 (2018) showed that that most limiting aspect of scanned probes could be automatically corrected. This is an important advance. It means that imaging and tip-based fabrication can at last be fully automated, parallelized and left to work unattended, freeing skilled physicists do other more rewarding work, AND, for the first time creating the realistic potential for atom scale manufacture of viable products.

Just placed on the arXiv is another paper by Wolkow’s group, again using machine learning to solve a very tough problem that had until now limited their progress. In “Autonomous Atomic Scale Manufacturing Through Machine Learning”, all the common defects seen on the silicon surface are recognized and avoided by machine learning methods. Ideal, defect free regions are automatically located within a target area. Also automatically, the probe then carries out a multi-atom fabrication process. The example given is of an atom-defined binary logic gate. The paper has been submitted to Nano Letters. arXiv:1902.08818

This new approach renders a ~1% defective substrate effectively perfect. Defects arte entirely avoided as is circuit failure due to pre-existing defects. Another step toward a manufacturable process.

Key dangling bond insights gained *before* all these new patterning tools came into play

Before all of these innovations were in hand, Wolkow’s team had been making headway toward atom-defined Si functional units for circuitry. In “Controlled coupling and occupation of silicon atomic quantum dots at room temperature”, Phys.Rev.Lett. **102**, 046805 (2009) cited 190 times, the team showed aspects of field controlled computing that were like those shown earlier by Lent, Porod, Snider and their colleagues at Notre Dame. The atomic system had many advantages: identical dots, charge traps were eliminated and the extreme small size created an extremely large splitting energy of the symmetric and antisymmetric states formed between dots. The latter effect allowed electronic state control to be observable at 300 K rather than 4K. Before publishing that work, a patent “Atomistic quantum dot” was filed. That patent, with all of its very broad claims, was granted in 2011.

Many new insights into single electron dynamics at DBs

More recently, amazing qualities of silicon dangling bonds were uncovered that had escaped attention till then.

In “Single-Electron Dynamics of an Atomic Silicon Quantum Dot on the H− Si (100)−(2× 1) Surface”, PRL 112, 256801 (2014), it was at last clearly shown that the silicon dangling bond could exhibit a well defined (localised) positive state in addition to the previously known neutral (1 electron) and negative (2 electron) states. Density functional theory (or rather its current implementation) incorrectly places the positive state in the VB rather than in the gap.

In “Scanning tunneling spectroscopy reveals a silicon dangling bond charge state transition”, New J. Phys. 17, 073023 (2015), a surprisingly abrupt, reproducible, current onset was observed in current- voltage spectra over certain dangling bonds. This was very puzzling to all in the community.

In the first all-electronic time-resolved (nanosecond temporal resolution, undiminished spatial resolution) STM measurement of a semiconductor, a beautiful explanation of the abrupt current onset and DB charge state change was found. It was shown that a near surface, non-ionized dopant, became field ionized at some critical negative sample bias. The sudden appearance of a positive ion (the dopant) caused a local downward band bending which in turn abruptly increased tunneling of electrons from the bulk through the depletion layer, directly to the DB. The reason the current passes exclusively through the DB (and not surrounding H-terminated Si, is because the DB provide a state to hop through. The several Angstrom longer path directly to the tip, without that stepping stone, is exponential disfavoured. Transport could be detected before the system relaxed to accommodate the applied field and as a result distinct ionization and neutralization rates of a single dopant were measured. Very cool. “Time-resolved single dopant charge dynamics in silicon”, Nature Comms. 7, 13258 (2016).

In a subsequent time resolved STM study together with a Green’s function transport model, a long standing puzzle about the nature of negative differential resistance at a single silicon atom was at last resolved (and previous, long standing explanations were eliminated). In “Time-resolved imaging of negative differential resistance on the atomic scale, PRL. 117, 276805 (2016), a robust negative differential resistance feature from a well defined species was identified as a many body phenomenon related to occupation dependent electron capture by a single atomic level. They measured all the time constants involved in this process and atomically resolved, nanosecond time scale images were presented to simultaneously capture the spatial and temporal variation of the observed features.

In “Resolving and tuning carrier capture rates at a single silicon atom gap state”, ACS Nano 11, 11732 (2017) Wolkow’s group reported tuning of the carrier capture events at a single dangling bond by varying the substrate temperature, doping type, and doping concentration. Such measurements were previously inaccessible. Time-resolved STM was employed to directly measure the carrier capture rates on the nanosecond time scale. A characteristic negative differential resistance feature was evident at dangling bonds on both n- and p-type doped samples. It was found that a common model accounted for both observations. Atom specific Kelvin probe force microscopy corroborated the IV study, giving the relative energetic positions of the DB’s charge transition levels. Further tuning was achieved by altering the majority carrier concentration of the system. Measurements made at higher temperature enabled thermionic carrier generation and the increase of rates. The first measurement of filling and emptying rates for the (0/+) level from the valence band have been determined. Finally, a target DB’s electronic

character was shown to be tunable in a predictable manner through Coulombic interactions induced by the placement of negatively charged DBs nearby.

Through these papers a new and deep understanding of the dangling bond's electronic properties has emerged.

In the last 2 years A leap forward when his new patterning tools came on-line

Binary atomic silicon logic, BASIL

Most recently, Wolkow achieved a major goal he set for himself about 15 years ago. He showed the first proof of concept binary atomic silicon logic functions, Nature Electronics 1, 636 (2018). At the same time, "Initiating and monitoring the evolution of single electrons within atom-defined structures", Phys. Rev. Lett. 121, 166801 (2018) was published. Multiple patents were filed in advance of publication. Here at last his work is extremely close to real proof of concept and even specialized commercial applications of his atomic electronic devices.

In the binary atomic silicon logic Nature Electronics paper the creation of a double well potential defined by two atoms is exactingly defined and characterised. A negative charge placed to one side causes the electron in the double well to sit to one side. On moving that electrostatic "input" to the other side, the electron moves to the other minimum accordingly. They defined a single beautiful bit in this way. Atomic force microscopy (and related Kelvin probe force microscopy) was used to measure the bias at which a single atom changes occupation by one electron. Atoms in different bias conditions show reconcilable differences in ionization potential. They were able to clearly show their "bit energy" is of order 200 meV. This is an ideal energy regime. 200 meV is sufficient confinement to ensure no loss of information by thermal buffeting, and is attractively small (unlike in today's technology is) so that excess energy need not be spent in the manipulation of bits (computing).

Moreover, unlike in CMOS where electrons are disposed of with each cycle of the clock, this field controlled approach endless reuses the same electrons over and over, saving energy in the process.

One figure in the Nat. Electronics paper shows a entity called a binary wire (proposed by Lent and colleagues at Notre Dame years earlier). Double well potentials, each with one electron, are aligned end to end. A bias in the form of a negative charge applied to the "left" terminus causes all the electrons to occupy the "right" side of their respective double well. The effect is shown to be bidirectional. This is amazing. State, and therefore information can be transmitted very fast and without consumption of conventional current. This could be a revolutionary advance. Estimates of power reduction of 100x compared to CMOS and clocking in the THz regime have been made.

Finally, in that paper they show the first binary atomic silicon logic gate. They actuate it with static charge inputs. A full truth table for a logical OR gate was shown. They argue it will soon be dynamically actuated when they wire it up with dangling bond conducting wires and that diverse gates and other entities will follow.

Wolkow is now extending this work to make an ultra low power yet ultra fast analog to digital converter in collaboration with Samsung in Austin Texas. It turns out that a dramatic power reduction is enabled by his technology when deployed in new hybrid analog/digital microprocessors that others have developed. The overall idea is that very fast and lower power vector multiplication can be done in analog. The bottle neck to practicality is fast, low power A to D. A very exciting, well aimed, real world, lucrative issue.

With Konrad Walus at UBC EE, arXiv:1808.04916 an open-source design and simulation tool for atomic silicon circuitry has been made available to all. His colleagues at Samsung are already using it. Wolkow hopes to have students around the world using the tool to design atomic circuitry. The tool accounts for the binary wire and logic gate already published while also showing designs expected to work for AND, NOT and more complex functions too.

An atomic electronic machine/simulator

"Initiating and monitoring the evolution of single electrons within atom-defined structures", Phys. Rev. Lett. 121, 166801 (2018) is a companion paper to the recent Nature Electronics Binary Atomic Silicon Logic paper. In that PRL they show the "free statistics" of a simple atomic ensemble that is an embodiment of a Ising-like Hamiltonian.

The position, and therefore energy, of electrons in multiple binary units show a collective evolution of state. While much remains to be done, it is clear from this first result that a ground state configuration when the electrons minimize repulsion, is most probable, and that excited states are seen more rarely. This is the essence of a Gibb's distribution. While it is very cumbersome and inaccurate to calculate a Gibbs distribution using Monte Carlo Markov Chain methods, this little machine simply creates a distribution automatically.

There is good reason to believe Wolkow can in this way make machines that are isomorphous with problems of great interest. One enormously interesting problem they can address is a neural network. While current popular methods – variants of simple contrastive divergence training on labelled data has spectacularly opened the door to machine learning for practical applications, there are many more problems requiring unsupervised learning and Gibbs sampling for training (Gibb's sampling enables optimal steepest descent for convergence of weights and biases) on unlabelled data.

With 1Qbit in Vancouver, Wolkow has entered into an agreement for designing a hardware (atomic) Gibb's sampler that will accelerate and provide power saving for neural network training.

A last note, on tool development and current commercial success

Wolkow has always been a builder of new instruments. For example, his home-made multiprobe STM was used to make the first determination of the resistance of a single atomic step on a silicon surface. A notoriously difficult measurement. The result was combined with state of the art transport theory to explain the quantum mechanical essence of scattering at a step. PRL. 112, 246802 (2014)

His reproducible (and in situ perfectly repairable) single atom tip is being commercialized with Bruker as mentioned earlier.

He has recently come upon a way – patents just filed – to solve another extremely challenging scanned probe related problem, that of “creep”. A new prototype, being discussed with three potential customers now, completely eliminates creep. Among other things, this means one can move the probe laterally to scan a new area and immediately collect warp-free useful images. This means greatly improved efficiency (more than a factor of 2 time saved). Multiple other applications, well beyond scanning microscopes, are planned. His scanner tech appears likely to provide another commercial success.

Wrapping up

Many important results and innovations. The goal of single atom precision technology and manufacturing was the highest ambition shared by many at the outset of the drive to nanotechnologies. He has achieved that to a substantial degree and has imagined applications that appear enormously important and with real prospects to succeed.