# The Quantum Initiative

## Energy in the 21st Century

Thomas Lee Elifritz
The Archimedes Group
221 East Main Street
Marshall, Wisconsin 53559
elifritz@charter.net
(608) 345-8891

Solving the atmospheric carbon crisis in the 21st Century requires the cessation of carbon combustion. Accomplishing this goal in a timely fashion will require optical absorption, reflection, transmission, modulation and attenuation surfaces utilizing innovative thin film technologies for insightful photo conversion processes, including the subsequent electromagnetic, electrochemical and thermodynamic energy conversion processes operating at large fractions of Carnot cycle efficiency and cascading into cogeneration pathways utilizing appropriately placed thermal insulation barriers and thermal masses.

Consider optical energy conversion processes involved in hypothetical universal energy conversion pathways, from the ultraviolet (UV) at ~ 3.1 eV, down through the optical at around 1.65~3.0 eV, then through infrared (IR) vibration and rotation at 0.001~1.65 eV and continuing through the microwaves, to radio waves, and alternatively, the Fermi level in quantum many-body systems, or the ground state in atomic and molecular systems. Our available reservoir of energy consists of solar white light, above and within the atmosphere, as a superimposed mixture of a spectrum of incoherent chromatic photons. This highly dispersed solar energy can be collected at a wide variety of wavelengths, converted into an electromotive force of mobile electrons, which automatically decays into the infrared by dissipation.

We now know those mobile electrons to be superpositions of both coherent and incoherent electronic states consisting of composite electron and hole pair structures, collective excitations of those entities, and the resulting composite bosons and fermions, subject to the constraints of the BCS-BEC crossover. Some of these states may become topologically protected at edges, surfaces, defects, dislocations and domain walls in structured condensed matter systems, and are relativistic near Dirac cones and points, and include Weyl points and line nodes and the Majorana and Weyl fermions that may thus be realized.

The domain of useful work that may be performed by these mobile electrons is thus vastly expanded over conventional metallic conduction, donor acceptor semiconductor physics and logical switching, and now includes controlled heat transfer and dissipation, conventional and quantum computing, and entirely new and efficient processes of plasmonics, magnonics, spintronics, orbitronics and Mottronics, and yet to be discovered emergent electromagnetic and chemical phenomena that are bound to arise.[1]

I propose an international quantum initiative to study the electronic, phase, orbital, spin, lattice and vibrational excitations of the discrete and condensed matter systems thought to be useful as optical, electronic and thermal media, at the quantum mechanical, electromagnetic and thermodynamic levels. Once a fundamental understanding of the quantum physics of available energy conversion pathways is achieved, this information can then be used to design and construct useful energy conversion devices. Once reduced to practice, any new and useful quantum energy conversion process and devices can then be further utilized to construct innovative implementations of new ultracold and near room temperature quantum simulators and quantum computers, that will be useful for the progressing quantum initiative. This strategy of immediate technological and device feedback, already being routinely performed in the ultra cold atomic gas laser cooling and trapping domain, can then be extended up to room temperatures.

The urgent near term imperatives of this new quantum initiative are room temperature thermoelectric energy conversion and high temperature superconductivity, since these regimes are fully expected to converge at somewhere near cryogenic temperatures in the near future. Demonstration of much more efficient solid state refrigeration would motivate and enhance the commercial funding of research and development in these specific areas, and would result in immediate commercially viable applications.

To properly frame this specific problem, I have suggested that the relevant photon energy and thermal temperature scales may be set by both the enthalpy of formation of water at roughly ~ 2.97 eV, and the triple point of water at 273 K, where the UV scale may be best represented by the high energy excited electronic states of the bismuth iodide molecule. This sets the ultraviolet cutoff at 2.9~3.1 eV, the third and fourth excited states of bismuth iodide (Fig. 1) marked by the 405 nm violet emissions of a gallium nitride (GaN) violet laser diode, or a frequency doubled gallium arsenide (GaAs) infrared laser diode. To get a sense of this scale of energy, the green to ultraviolet region of the optical spectrum is roughly one hundred times more energetic than the thermal energy (temperature) of water in the liquid state.

The ultimate goal of modern day energy conversion is, of course, the freezing and boiling of water, and the photochemical and electrochemical dissociation of water into molecular hydrogen and oxygen, and the subsequent recombination of these cryogenic compounds, releasing water, heat and energy, either thermal, electrical or directly into momentum by the use of reaction engines formally known as rockets. Like the messy state of diffuse light, photodissociation of water is also a messy reaction, involving the cleaving of two hydroxide bonds and recombination of the atomic hydrogen and oxygen with ionized hydroxyl intermediates.[2,3] Molecular hydrogen and oxygen are cryogenic liquids, so without some clear solid state thermoelectric or thermomagnetic energy conversion pathways, their storage is problematic. Clearly liquid hydrogen and oxygen can be stored and transported in cryogenic dewars, but condensing them into the liquid state requires cooling to roughly 20 K and 90 K respectively, which is challenging.

The most promising element by far to begin the investigation of quantum energy conversion is bismuth. Calculated theoretical $zT$ efficiency of hexagonal bismuth monolayers is estimated to be in the range of around 3-4,[4] easily high enough to jump start thermoelectric energy conversion devices for any of the new bismuth based spin orbit coupled topological insulators and superconductors with exotic surface and edge states and line and point singularities. Isolated bismuth ions in reduced states, embedded in borosilicate and rare earth glasses[5] have well known infrared fluorescence emissions that are useful in long distance broadband fiber communications. It was just predicted that hexagonal bismuth halide[6] monolayers on silicon, or some other lattice compensated insulating surface, will display precisely the topologically protected edge states desired for propagation of coherent electrons at room temperature.[7,8] High density bismuth iodide,[9] where the one-dimensional polymerized zig-zag wire geometry of the lattice is defeated by the breaking of the bismuth-bismuth metal-metal bonding, is expected to become an array of isolated $Bi^+$ ions embedded in a sea of highly polarizable iodine ions, allowing the excited third and fourth electronic states to be stable within infrared vibrational fluctuations at ~ 2.9 ~ 3.1 eV.[10] This system of bismuth iodide is accessible by simple violet laser excitation at a wavelength of 405 nm.

I intend to use polymeric one dimensional pure bismuth iodide, $Bi_4I_4$, and possibly $Bi_{14}I_4$, as feedstock for the physical and chemical deposition (adatom adsorption and desorption), and the pulsed laser[11] deposition (3 eV, XUV and soft X-rays) of the bismuth halide monolayers. Laser assisted molten salt quenching of bismuth iodide, using argon gas gloveboxes, evacuated quartz or Pyrex glass tubes with tungsten electrode plugs and 405 nm laser excitation, will also demonstrate the fundamental kinetics and energetics of the systematic and structured making and breaking of bismuth-bismuth metal-metal bonding necessary to implement geometrically arrayed bismuth monolayer islands, wires and channels on clean insulating substrates, without resorting to electrochemical underpotential deposition on gold.

The orbital tuning of hexagonal two dimensional monolayers and the bulk three dimensional lattices necessary for the creation of nontrivial and topologically protected edge and surface states, are more amenable to intercalation of univalent dopant ions, while divalent species result in more complex and inhomogeneous, laminated and phase separated compounds that are now well known for these effects, including but not limited to bismuth tellurides, selenides, sulfides, antimony tellurides and selenides, arsenides, pnictides, nitrides – group V compounds quite generally, as is to be expected on principles. These effects may be quite generally referred to as generic to compounds called group V alkali halides. Considering the hydrogen atom as both an alkali and a halide, and considering the group V elements as both oxidation and reduction agents, then clearly alkali metal ammonia solutions and iodobismuthine[9] are the unique low and high molecular weight 'metal in polar solvent' terminations across this spectrum, with solvated electrons in water as being the most unique and useful manifestation of this phenomenon.

On the other hand, a compound as simple as hydrogen sulfide, $H_2S$, possibly the most undesirable of all conceivable technological molecules, is now known to dissociate and polymerize[12] at enormously high pressures, where it subsequently becomes an ordinary superconductor at extremely high temperatures.[13] Rather unsurprising then is the recent identification of the bismuth sulfides as unusual superconductors and molybdenum and tantalum disulfides, etc. have emerged as unique platforms for orbital electronics. Working devices are more reliably engineered by the judicious use of chalcogenide divalent elements, such as the ubiquitous bismuth tellurides and bismuth selenide alloys and the antimonides, BiSbSeTe.[14]

The ideal realm to study dilute systems of rare earth atoms and bismuth nanoparticles are borosilicate transparent glasses,[5] which represent the clearest method forward in designing diffuse light collection devices and plasmonic cathodic fluorescence schemes. The varying bismuth nanoparticle sizes produce varying surface excitations which can be coupled to the ground state excitations of the isolated bismuth ions and atoms, dimers, trimers, etc.[15] Using selected rare earth elements, broadband optical absorption and emission directly integrated into novel photonic to electronic energy conversion pathways driving quantum computational and superconducting digital circuitry *at the subnanoscale*, becomes possible.

The engineering of new technological applications in this field will involve tuning both the electron-phonon and electron-lattice interactions on the one hand, and the electron-electron interactions that inevitably accompany strong electronic correlations in the intercalated or doped solids or solutions. Balancing these two competing and cooperating phenomena is required to create the desired effects, where a variety of tunable parameters must be considered such as hydrostatic and chemical pressure, temperature, composition, structure, order, disorder, excitation, coherence, decay and then dissipation.

Whereas optimization of BCS superconductivity requires low atomic weight, high phonon frequencies, strong electron-phonon coupling and high density of states at the Fermi level, for instance – hydrogen, BECs require strong electron interactions and correlation resulting in strong attractive pairing energies, effective Coulomb screening, high charge carrier density and low effective masses for (de)localization. These conflicting constraints generally result in lattices with a propensity for phase separation behavior in which charge carriers residing on or passing through phase boundaries take on exotic characteristics.

Driving phase coherence coupled with charge mobility at room temperature and ambient pressure will by fundamental physics necessarily involve electrons, holes, protons, impurities, defects and vacancies. At these energy scales - polarons, bipolarons, excitons, polaritons and their composite excitations and quasiparticles can be controlled by engineered inhomogeneities within atomic and molecular systems. What these engineered solid state and condensed matter devices and systems will ultimately resemble, to what purposes they will be applied, or how they will be used in the future – still remains to be seen. However, this is clearly required if we intend to reverse our planetary carbon contamination problem.

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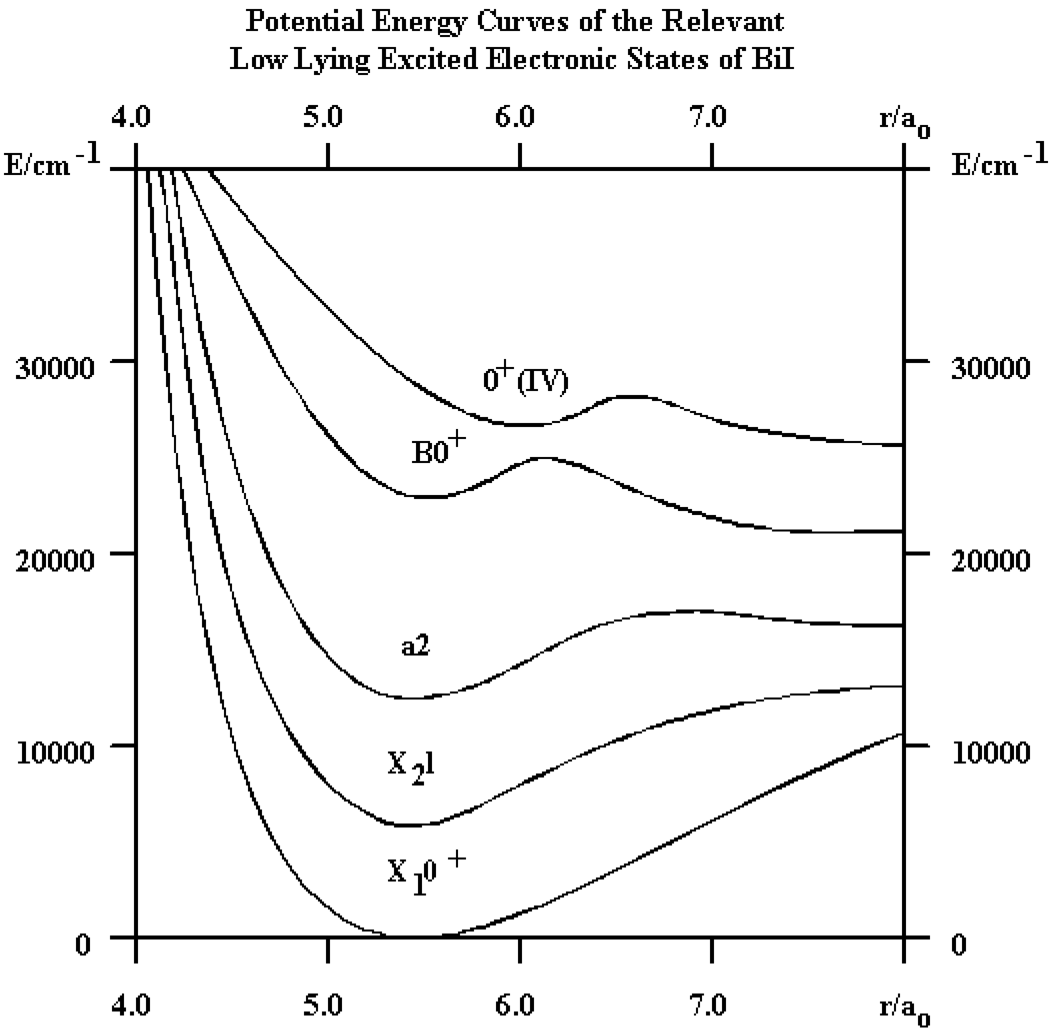

**Figure 1**: Potential energy curves of the relevant low lying excited electronic states of BiI, showing the hypothesized infrared active metastable III and IV excited electronic states of the bismuth iodide ions.

Adapted from Alekseyev, *et al.*, Chem. Phys., 198, 333-344 (15 September 1995), doi:10.1016/0301-0104(95180-V)00

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