American Mineralogist, Volume 95, pages 669–670, 2010

Acceptance of the Dana Medal of the Mineralogical Society of America for 2009

Ronald E. Cohen

Geophysical Laboratory, Carnegie Institution, 5251 Broad Branch Road N.W., Washington, D.C. 20015, U.S.A.

First, I express my appreciation to the MSA; this means a lot to me. Attention is often paid to scientists at the head and the tail of their careers. We think of young scientists as needing special attention and appreciation to help get their careers started. Giving tribute to our esteemed colleagues for a lifetime of research and service is also time honored and proper. But for the person still slogging through the middle of one's career, fighting daily frustrations, always finding it difficult to make progress as rapidly as desired, daily facing technical and conceptual roadblocks, the appreciation of one's colleagues is especially appreciated. The beginning of the journey is always exciting, though filled with trepidation, and the end is satisfying, one hopes, but the day-to-day trip can sometimes be grueling, and a little encouragement goes a long way. I hope MSA will consider this award for any deserving member of MSA, regardless of previous awards.

I want to thank Russell Hemley for his kind words, and also for his guidance and encouragement over the years. I owe the direction my career and research has taken almost entirely to Rus. We were next-door neighbors in the graduate dorm at Harvard, and the day that Rus showed me phonon dispersion curves computed using the Gordon-Kim model, with no data, it opened my eyes to a new world of possibilities. Rus applied to the Naval Research Lab and the Geophysical Lab for post-doc positions, and went to the Geophysical Lab. I followed his lead and went the other way, to NRL to work and learn from Larry Boyer. I started as a geologist interested in fieldwork and experiments, under the tutelage of Jim Thompson, Jim Fred Hays, and Dave Walker, and ended up a theorist working on superconductivity, ferroelectricity, and high-pressure physics. I was hired as a staff physicist at NRL and had productive years there working under Barry Klein. I learned a lot from Warren Pickett, Henry Krakauer, and other computational physicists. I did maintain my interest and research into applications of first-principles theory to geophysics, and my contacts with Earth science at meetings and my friends at the Geophysical Lab. When Charlie Prewitt offered me a staff position at the Geophysical Lab, I felt it was an offer I couldn't refuse, where I have been free to do research without concern for disciplinary boundaries. I want to thank the Carnegie Institution for supporting me and providing a nurturing environment for my research since I arrived there in 1990. I also want to especially thank the postdocs and students who have worked with me, and without whom much less could have been accomplished.

When I started, the idea of first-principles computations, particularly total energy calculations, was new, and only rather simple materials had been studied at all. In Earth science, there was only Mark Bukowinski using self-consistent density functional theory based first-principles methods. It is hard to believe now the hostility often expressed then against first-principles theory. Even now one occasionally runs across a hostile experimentalist, but generally theory is accepted as a complementary tool to help us understand Earth and other materials, and the Earth. Now there are hundreds of new density functional studies published each month, and many mineral physicists and geochemists use these methods. Experimentalists are starting to routinely use theory to make predictions to guide their experiments, and I think every young experimentalist in mineralogy, mineral physics, or geochemistry should not only understand theory well enough to critically read theory papers, but also learn how to use one of the community electronic structure codes such as ABINIT.

The Dana award is a mid-career award, which is nice, because I am not done yet! As DFT methods became more commonly used, I started to consider the second half of my career. When I started out, what I was doing was new, but now DFT methods are often applied. So I have started learning new techniques, which hold the promise of much greater accuracy, at the cost of greater

0003-004X/10/0004–669$05.00/DOI: 10.2138/am.2010.555

computational complexity, and dealing with the remaining difficult problems of open shelled systems, such as the geochemically all-important transitional metal ions such as iron.

I want to thank my wife Kathy and children Daniel, Jacob, and Rebecca for coming to Davos, and putting up with all of my travel in particular. Unfortunately my parents are no longer around, and my mother had expressed her desire to come here for this occasion, but passed away October, 2008, but I want to express my appreciation to my parents for teaching me to think for myself.

Now, I want to use this opportunity to say a few words about computational theory, and its place in mineralogy, mineral physics, and the materials sciences. Theory does not replace experiment, but it is now possible to place a high reliance on some first-principles methods to the extent that problems with experiments can be detected, and properties can be reliably predicted in the absence of data. We should not be surprised that computational theory can be very accurate. The underlying theory, quantum mechanics, is exact, and we know that fundamental physical quantities, such as the fine-structure factor, can be computed accurately to many significant figures. The problem for solids is that although we can compute total energies quite accurately, the chemical and physical effects of interest, such as transition temperatures and pressures, elasticity, etc., are on quite small energy scales, and most of the energy is not chemically interesting at ordinary conditions. Nevertheless, great progress has been made, and relatively simple approximations to the many-body electronic interactions have proven quite accurate after testing on many thousands of systems over the last decades.

The main approaches to solid and fluids properties are based on density functional theory (DFT), which is an exact theory for ground state properties. However, the exact density functional is not known in a useful form. Fortunately, the simplest approximation, known as the local density approximation (LDA), works amazingly well. The LDA should be easy to understand by metamorphic petrologists and geochemists, as it is like the idea of local equilibrium. The LDA assumes that the complex many-body electronic interactions at each point in space in a material are just like those in a uniform electron gas with the same density as the density at that point. It has been shown that the accuracy of the LDA is largely due to compensating errors in the many-body interactions; nevertheless it has proved very useful. Extensions to the LDA include gradients in the charge density, such as the generalized gradient approximation (GGA), of which there are several flavors.

In spite of its general success, there are cases where DFT within the LDA or GGA fails, which especially impacts applications in mineralogy and Earth science. In particular, transition metal ions in oxides and silicates are not properly treated, and crystals such as FeO, for example, are incorrectly computed to be metals, whereas they are insulators. DFT can be patched up with LDA+U or other methods, but results are model dependent, and not always predictive. Even non-exotic materials like silica are qualitatively wrong within the LDA, which gives stishovite as the ground state structure. We can either live with these failures, or look ahead to methods that, although much more computationally intensive, are more reliable.

Quantum Monte Carlo (QMC) can give extraordinary accuracy, and it is improving rapidly due to the hard work of a small group of experts who are developing methods and codes and making these publically available to other researchers. QMC fixes the above deficiencies at tremendous computational cost. However, QMC is perfectly parallelizable, and the rapid growth in parallelization possible, and especially the growth in GPU type architectures, will make QMC as tractable as DFT is now. So it is a good thing to learn about!

I have always said that theory is useful to: (1) help guide experiments; (2) help interpret experimental results; and (3) provide estimates when no data are yet available. Theory and computation should be part of the training of all young researchers, as they will be playing a more and more important role in the future. To quote the 1959 Edward D. Wood Jr. movie "Plan Nine from Outer Space": We should all care about the future, because that is where we will be spending the rest of our lives!