Recent Developments in Computing the Properties of Atoms in Materials

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The recent advances in computational power are making it ever more practical to use quantum chemistry methods to study complex materials. A key challenge is to extract meaningful insights from the results of these computations. Although net atomic charges, bond orders, and magnetic moments are widespread chemical concepts, their computation requires specialized methods. This talk will summarize recent developments in Density Derived Electrostatic and Chemical (DDEC) atomic population analysis. The latest generation of this method, called DDEC6, offers substantial improvements in accuracy and computational cost compared to prior generations. The DDEC6 method assigns net atomic charges (NACs), atomic spin moments (ASMs), bond orders, atomic multipole moments, polarizabilities, and dispersion coefficients using only the total electron and spin distributions of the material as inputs. A key advantage of this approach is that the atomistic descriptors have been optimized to accurately reproduce both the chemical states of atoms in materials and the force fields surrounding the material. This makes them ideally suited both for studying the chemical properties of materials and for constructing force-fields used in classical molecular dynamics or Monte Carlo simulations. To assess the accuracy of this approach, comparisons of computational to experimental results will be presented for a broad range of periodic and non-periodic materials.

Brief bio: In 1994, Manz received a bachelor of science in Chemical Engineering from The University of Toledo in Toledo, Ohio. He received M.S. (1998) and Ph.D. (2009) degrees in Chemical Engineering from Purdue University in West Lafayette, Indiana. His Ph.D. work focused on computational modeling of olefin polymerization catalysts. From 2008 to 2012, he worked as a research scientist (post-doc) in Prof. David Sholl's group at Georgia Institute of Technology in Atlanta, Georgia. From 2012 to present, he is working as an assistant professor in Chemical & Materials Engineering at New Mexico State University. His research group develops new computational methods and uses computational chemistry to design new materials. In 2016, he received the NSF Career Award.