Interatomic Delocalization in Solids Under Pressure

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Bader's localization and delocalization indices (DIs) measure interatomic electron localization and electron sharing. At zero pressure, DIs between covalently bonded atoms are similar to the bond order. However, DIs exist between any pair of atoms in the system, which means that they can be used to measure electron delocalization in systems where van der Waals, ionic, or metallic bonding is dominant. For this reason, DIs rank among the most popular real-space indices used to elucidate the nature of a chemical bond. In this talk, I will present a new method that has been implemented in the critic2 program that allows the efficient and accurate calculation of DIs in solids. This new method opens up a new avenue for the study of chemical bonding in materials under pressure. The behavior of DIs with pressure in several model materials is examined.