Video abstract transcript:

Hello. I am Dr. Thomas Manz from New Mexico State University. This is a video abstract of "Introducing DDEC6 atomic population analysis: part 3. Comprehensive method to compute bond orders".

Bond order quantifies the number of electrons exchanged between two atoms in a material. Bond orders help us understand chemical reactivity and material properties.

Now let's compare four strategies to compute bond orders. In strategy one, bond order is computed from the difference in bonding and antibonding orbital occupancies. However, strategy one does not work for stretched bonds. In strategy two, the bond order is computed from the electron and spin density distributions. However, prior methods incorrectly assumed constant bond-order-to-overlap ratio. My new method described in the paper fixes this problem. In strategy three, bond order is computed from the first-order density matrix. However, strategy three gives inconsistent results, because different quantum chemistry methods give vastly different first-order density matrices. Strategy four partitions the exchange-correlation hole among atoms. However, strategy four is computationally expensive, because its number of components scales as the number of basis functions to the fourth power. Also, the existing strategy four gives a bond index that is numerically different from the bond order.

My method is based on DDEC6 partitioning that assigns atomic electron and spin distributions to each atom in the material. The paper explains why this partitioning is optimal for computing bond orders.

In this plot, the blue curve shows the total computational time for DDEC6 partitioning including core and valence electron partitioning and bond order analysis increases linearly with increasing number of atoms in the unit cell. The red curve shows the total required random access memory also increases linearly. The orange curve shows the required computational time for just DDEC6 bond order analysis. These results show DDEC6 bond orders can be readily computed for materials containing many thousands of atoms in the unit cell.

Various molecules, organometallic complexes, solids, nanostructured materials, and spin multiplets were studied. These included materials with no magnetism, collinear magnetism, and non-collinear magnetism. Bonding types included covalent, polar-covalent, metallic, aromatic, electron-deficient multi-centered, hypercoordinate, dative, hydrogen bonding, and stretched bonds. These results show the method is consistently accurate for a wide range of materials and bonding types.

Special thanks to the National Science Foundation and XSEDE for supporting this research.