

The Role of Many-Body Dispersion Interactions in the Racemic and Enantiomeric forms of Crystal Alanine. FARREN CURTIS,

Physics and Engineering Physics, Tulane University, New Orleans, LA, ALEXANDRE TKATCHENKO, Fritz Haber Institute of the Max Planck Society, Berlin, Germany, NOA MAROM, Physics and Engineering Physics, Tulane University, New Orleans, LA, Polymorphism in molecular crystals is a phenomenon where crystals of the same molecular composition can crystallize in more than one structure. Different polymorphs of the same crystal may be extremely close in energy but may possess vastly different physical properties. It is well-known that hydrogen bonding and van der Waals (vdW) interactions play a large role in the formation and stability of polymorphic molecular crystals but these interactions are absent from standard semi-local Density Functional Theory (DFT) functionals in first-principles calculations. Recently, there has been much progress on dispersion-corrected DFT methods that use various vdW and dispersion corrections on top of a standard DFT calculation. These methods have demonstrated unprecedented accuracy in calculating the the structures, relative stabilities, and even anisotropic elastic properties of molecular crystals [Angew. Chem. Int. Ed. 52, 101002 (2013), PRL 113, 055701 (2014)]. Pairwise dispersion methods, such as the Tkatchenko-Sheffler (TS) [PRL 102, 073005 (2009)] method, apply a pairwise correction to approximate the leading term in the vdW energy. Many-body methods such as MBD [Phys. Rev. Lett. 108, 236402 (2012)] or MBD@rsSCS [J. Chem. Phys. 140, 18A508 (2014)], although computationally expensive, provide even higher order corrections to the vdW energy. In this work we look at two polymorphs of the amino acid Alanine which forms either enantiomeric (L-alanine) or racemic (DL-alanine) crystals. These two polymorphs are a challenging case for dispersion methods because one needs a highly accurate description of the energetics in order to calculate their relative stability. We compare the results of PBE, PBE+TS, and PBE+MBD@rsSCS for the calculation of the structure, relative stability, and certain elastic properties of these crystals.