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Van der Waals materials: what is the origin of the disagreement between ab initio calculations and experiments? LOREDANA VALENZANO, WARREN PERGER, JACKSON CRISWELL, WILLIAM SLOUGH, Michigan Tech Univ — The robust prediction of accurate physical properties for molecular solids from first-principles calculations continues to present a significant challenge across a wide variety of scientific disciplines. Comparison between computed and experimental values for physical properties derived from differences between states is often promising (such as bulk modulus), however the result is disappointing for absolute values (such as density). Accurate ab initio calculations describe physics occurring at zero Kelvin; but, properties evaluated experimentally are mostly reported at room temperature. Therefore it should hardly be surprising that ab initio results differ dramatically from experimentally measured values. We show how the results from a calculation at zero Kelvin may be compared to experimental values at higher temperatures, helping to foster a stronger linkage between computational and experimental work on systems such as energetic and pharmaceutical materials and metal-organic frameworks in interaction with guest molecules. Among others, investigated behavior comprises mechanical (elastic constants) and vibrational (infrared and Raman spectra) properties. The computational approach adopted, takes into account van der Waals long-range dispersion interaction through an empirical "a posteriori" approach, appropriately fitted to investigate solid materials.

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