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Active Pharmaceutical Ingredients: Prediction of Physical-Chemical Properties from First Principles LOREDANA VALENZANO, Michigan Technological University — Polymorphism in active pharmaceutical ingredients (APIs) plays a crucial role both for medical and intellectual property concerns but despite ongoing efforts, experimental and computational investigations of the existence and the physical-chemical properties of the same compound in different forms is still an open question.While comparison between computed and experimental values for properties derived from differences between states is often promising (such as bulk modulus), results are disappointing for absolute values (such as density). Quantum mechanical computational methods describe the systems at 0K, experimentally properties are often evaluated at room temperature. Therefore it is not surprising that results determined from first principles dramatically differ from those obtained experimentally. By applying a quantum mechanical periodic approach that takes into account long range London dispersion forces fitted for solid materials, and by imposing different cell volumes corresponding to different thermodynamic conditions, we show how results from calculations at 0K (structures, vibrational spectra, elastic constants) may be compared to experimental values at higher temperatures, helping to foster a stronger linkage between computational and experimental work on systems such as APIs. Where experimental results are not available, our work represents an innovative approach in addressing the properties of APIs. Our results can also serve as foundation for the developing of new force fields to be adopted within a multi-scale computational approach.

Loredana Valenzano
Michigan Technological University

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