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Van der Waals Interactions in Aspirin ANTHONY REILLY, Cambridge Crystallographic Data Centre, ALEXANDRE TKATCHENKO, Fritz-Haber-Institut der MPG — The ability of molecules to yield multiple solid forms, or polymorphs, has significance for diverse applications ranging from drug design and food chemistry to nonlinear optics and hydrogen storage. In particular, aspirin has been used and studied for over a century, but has only recently been shown to have an additional polymorphic form, known as form II. Since the two observed solid forms of aspirin are degenerate in terms of lattice energy, kinetic effects have been suggested to determine the metastability of the less abundant form II. Here, first-principles calculations provide an alternative explanation based on free-energy differences at room temperature. The explicit consideration of many-body van der Waals interactions in the free energy demonstrates that the stability of the most abundant form of aspirin is due to a subtle coupling between collective electronic fluctuations and quantized lattice vibrations. In addition, a systematic analysis of the elastic properties of the two forms of aspirin rules out mechanical instability of form II as making it metastable [A. M. Reilly and A. Tkatchenko, Phys. Rev. Lett. 113, 055701 (2014).]

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