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**An ab initio study of crystalline and molecular biotin**[1] MILO LIN, Department of Physics, California Institute of Technology, DAVID PRENDERGAST, GIULIA GALLI, Lawrence Livermore National Laboratory — The protein cofactor, biotin, has been studied due to its importance in human metabolism and its ability to selectively bind to proteins such as avidin. Understanding the selectivity of biotin from an analysis of its structural stability will help in developing new bio-sensor engineering applications. Experimental analysis of the structure of biotin is typically carried out using x-ray diffraction from crystalline samples. We analyze the differences in energetic, structural, and dynamical properties of biotin in its experimentally determined crystalline form and in its proposed molecular form. Using first principles density functional theory calculations we determine the cohesive energy of the crystalline phase. These calculations explore the limitations of density functional theory, under the generalized gradient approximation, in describing hydrogen-bonding and long-range order in molecular crystals. We analyze the structural stability of both crystalline and molecular phases by calculating the phonon spectrum. Particularly soft modes in the molecule are related to its change in conformation in transforming from the molecular to the crystalline phase.

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