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Role of anharmonic contributions for the elasticity of ice MIRA TODOROVA, LARS ISMER, JÖRG NEUGEBAUER, Max-Planck-Institut fuer Eisenforschung GmbH, Duesseldorf — Water, one of the simplest molecules in chemistry, forms a liquid and solid phase with features essential to live and environment. Many of these can be attributed to hydrogen bonding, but that does not mean that they are fully understood. Ice should be an easier material to understand, because its molecules are arranged on a regular lattice. Yet even the determination of such basic properties as the bulk modulus and the elastic constants proves to be a challenge. Using first principles calculations we investigate the bulk properties of hexagonal ice. Our initial density-functional theory calculations (GGA-PBE level) yield values, which are much too high when compared to experiment. Even though the consideration of thermal effects within the quasi-harmonic approximation leads to a qualitative agreement between measured and calculated quantities, such as the linear expansion coefficient, ice remains much too hard. The large overestimation of the ice' softness demonstrates the importance of anharmonic contributions, which will be shown to be crucial and lead to a dramatic reduction of the bulk modulus and the elastic constants.

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