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Anharmonic vibrational properties of solids and the metallization of solid helium BARTOMEU MONSERRAT, University of Cambridge, NEIL D. DRUMMOND, Lancaster University, CHRIS J. PICKARD, University College London, RICHARD J. NEEDS, University of Cambridge — We describe a firstprinciples method for the calculation of anharmonic vibrational properties in solids. The method is based on a principal axes mapping of the Born-Oppenheimer energy surface and the vibrational self-consistent field scheme, and it allows us to calculate, amongst other quantities, the anharmonic free energy, the band gap renormalizations due to electron-phonon coupling, and the vibrational stress tensor. We exemplify the method by determining the effects of electron-phonon coupling and thermal expansion on the metallization of solid helium. Our results have implications for the cooling of white dwarf stars and suggest a revision of current lower bounds to the age of the Universe as determined within cosmochronology.

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