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Lattice Dynamics of Cu_2O: Bulk and (110) Surface KLAUS-PETER BOHNEN, ROLF HEID, Forschungszentrum Karlsruhe, IFP, ALOYSIUS SOON, CATHERINE STAMPFL, School of Physics, University of Sydney — A number of theoretical studies have been carried out in the past to investigate the stability of various surface oxides for the O/Cu system however despite the fact that catalytic processes usually proceed at elevated temperatures stability at finite temperatures has never been studied for these systems. Modern ab-initio methods however allow for the determination of the lattice dynamics and the phononic contribution to the free energy. Using density functional perturbation theory we have studied the lattice dynamics of Cu_2O-bulk as well as $Cu_2O(110)$. In calculating the free energy as function of lattice constant we obtained for the bulk a negative thermal expansion up to roughly 300 K in excellent agreement with experiments. This is due to anomalous mode Grüneisen parameters for vibrational modes in the low energy regime. Due to the anomalous behavior of the mode Grüneisen parameter the bulk system is highly unstable against variations of the lattice constant by more than 2%. To investigate the stability of the O/Cu surfaces we have investigated the lattice dynamics of $Cu_2O(110)$ as a prototype. Despite a large number of low lying modes no instability has been found. These calculations allow also for the O/Cu system for the first time for a realistic estimation of the surface-free energy which is important for the determination of surface thermodynamic properties.

Klaus-Peter Bohnen
Forschungszentrum Karlsruhe, IFP

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