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Lattice Dynamics of RuO_2: Bulk and (110) Surface KLAUS-PETER BOHNEN, ROLF HEID, Forschungszentrum Karlsruhe, IFP, OMAR DE LA PENA SEAMAN, Department of Applied Physics, CINVESTAV-Merida — Although RuO_2 has been studied as a prototype catalyst for CO oxidation no careful study of the lattice dynamics for this material has been presented so far. Using modern ab-initio methods we obtain the phonon dispersion and the generalized density of states (GDOS). Inelastic neutron-scattering experiments allow for an experimental determination of the GDOS. In contrast to what is known from structural studies, we find that the local-density approximation gives a much better description of the phonon spectrum than the generalized gradient corrected form. This is also consistent with Raman measurements. Besides the bulk we have also studied the lattice dynamics for the (110) surface. Our calculations indicate an instability over a large range of the BZ. Unfortunately, no complete experimental phonon study of this surface has been carried out so far. Consequences for the structure of the (110) surface will be discussed.

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