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Anharmonicity in complex oxides: case of VO_2[1] JIAWANG HONG, OLIVIER DELAIRE, JOHN BUDAI, Oak Ridge National Laboratory, OLLE HELLMAN, Linkoping University, Sweden — Harmonic and quasi-harmonic models of lattice dynamics are widely successful in explaining thermodynamic properties of materials, including in complex oxides. However, in some cases, strong anharmonicity can critically affect physical properties, and a (quasi) harmonic model is not sufficient to capture these important features. In this talk, we present the results of ab initio molecular dynamics studies of anharmonicity in VO_2. Our simulations provide good agreement with measurements of phonon dispersions and diffuse scattering. Other implications of strong anharmonicity will also be discussed.

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