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**Heat Capacity of ZnO: Isotope Effects** MANUEL CARDONA, Max-Planck-Institut für Festkörperforschung, JORGE SERRANO, European Synchrotron Radiation Facility, REINHARD K. KREMER, GISELA SIEGLE, Max-Planck-Institut für Festkörperforschung, ALDO H. ROMERO, CINVESTAV, Departamento de Materiales, Unidad Querétaro, RUDOLF LAUCK, Max-Planck-Institut für Festkörperforschung — We have measured the heat capacity of zinc oxide for several single crystals with different isotopic composition in the 5 – 350 K temperature range. In order to analyze the dependence of the heat capacity on the isotope mass of the oxygen and zinc atoms, we have performed first-principles calculations within the harmonic approximation. The Zn mass affects mainly the acoustic phonons, thus leading to isotopic effects on the heat capacity mostly at low temperatures, whereas the O mass affects mainly the optic phonons, which become thermally active at higher temperatures. This behavior is reproduced quantitatively by the calculations, and is also in agreement with theoretical predictions reported for wurtzite GaN, an isostructural semiconductor. The possibility of using these data to obtain the density of phonon states projected on the corresponding atoms will be discussed.

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