

Dielectric constants of Zr silicates: A first-principles study

G.-M. Rignanese, F. Detraux, and X. Gonze

*Unité de Physico-Chimie et de Physique des Matériaux, Université Catholique de Louvain,
1 Place Croix du Sud, B-1348 Louvain-la-Neuve, Belgium
Research Center on Microscopic and Nanoscopic Materials and Electronic Devices (CERMIN),
Université Catholique de Louvain, B-1348 Louvain-la-Neuve, Belgium*

Angelo Bongiorno and Alfredo Pasquarello

*Institut de Théorie des Phénomènes Physiques (ITP),
Ecole Polytechnique Fédérale de Lausanne (EPFL),
CH-1015 Lausanne, Switzerland
Institut Romand de Recherche Numérique en Physique des Matériaux (IRRMA), CH-1015
Lausanne, Switzerland*

Abstract

Using density functional theory, we compute the optical and static dielectric constants for a set of Zr silicates modeled by various SiO_2 crystals, with Zr atoms substitutional to Si, and by an amorphous structure. We then derive a microscopic scheme that relates the dielectric constants to structural units centered on Si and Zr atoms through the definition of characteristic parameters. Applied to amorphous $(\text{ZrO}_2)_x(\text{SiO}_2)_{1-x}$, these schemes describe the observed dependence of the dielectric constants on the Zr concentration and highlight the role of ZrO_6 units.