Theoretical modeling of carbonate minerals in the WURM project

EMA BOBOCIOIU[1], EUGENIA VASILE[1] AND RAZVAN CARACAS[12]

[1]Ecole Normale Supérieure de Lyon, Laboratoire de Géologie de Lyon, Lyon, France
[2]CNRS

The Raman spectra of the majority of simple and complex carbonate minerals are determined using density functional perturbation theory in the ABINIT implementation and made available on the WURM website (http://wurm.info). Most carbonates have rhombohedral, i.e. calcite-like, or orthorhombic, i.e. aragonite-like, structures. Most spectra are computed at the theoretical 0GPa pressure and at the experimental density at ambient conditions. We also study in detail the Mg⇔Ca substitution and the order-disorder relations along the magnesite – dolomite – calcite series.

We find that all the Raman spectra are dominated, as expected, by the stretching modes of the planar CO_3 groups. The low-frequency modes are dominated by the heavy cations. Their degeneracy is directly determined by the symmetry of the structure. We performed a detailed comparative study to be able to identify identification trends. We determine peak position dependence on the Mg/Ca ratio and order in the $(Mg,Ca)CO_3$ series.

Finally we compute C and O isotope fractionation patterns between various carbonate polymorphs. We also compute their relative stability, and the hydration energies.