

## Density Functional Calculation of Raman Intensity in High Pressure Phases of TiO<sub>2</sub> crystal

D. Kirin<sup>1</sup>, I. Lukačević<sup>3</sup>, S.K. Gupta<sup>2</sup>, P.K. Jha<sup>2</sup>

<sup>1</sup> *Ruder Bošković Institute, Bijenička c. 54, 10002 Zagreb, Croatia*

<sup>2</sup> *Department of Physics, University of Bhavnagar, Bhavnagar, India*

<sup>3</sup> *Department of Physics, J.J Strossmayer University, 31000 Osijek, Croatia*

Intensity of Raman lines are important part of the information contained in the vibrational spectra of crystals. Due to the changes in the crystal structure as a response to external perturbation (pressure, temperature) the frequencies, as well as, intensities of Raman active modes change.

We have calculated Raman spectra of different crystal forms of TiO<sub>2</sub> crystal [1] as a function of pressure. The ABINIT density functional program package [2] are used for the calculation of vibrational frequencies and intensities of Raman bands. The values given by calculations are in a fair agreement with the observed positions of phonons as a function of pressure. The possibility to use Raman intensities as additional tool in the study of phase transitions is discussed.

[1] K. Legarec and S. Desgreniers, *Solid State Comm.* 94 (1995) 519–524.

[2] The ABINIT code is a common project of Universite Catholique de Louvain, Corning, Incorporated and other contributors ([www.abinit.org](http://www.abinit.org)).