MMPS 19 **Oral**

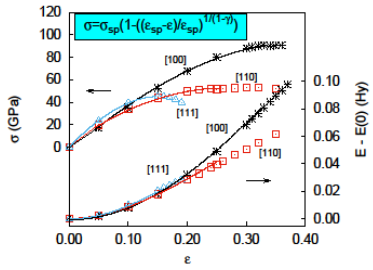
Impact of Stress on Structural and Stability of Prototype Ionic Materials: Spinodal Equation of State (3D-SEOS)

Hocine Chorfi*[1,2], Álvaro Lobato [1,3], Fahima Boudjada [2,4], Miguel A. Salvadó [1], Ruth Franco [1], Valentín G. Baonza [3,5] and J. Manuel Recio [1]

1 MALTA-Consolider Team and Departamento de Química Física y Analítica, Universidad de Oviedo, E-33006 Oviedo, Spain; zahraoviedo@gmail.com (H.C.); a.lobato@ucm.es (Á.L.); mass@uniovi.es (M.A.S.); ruth@uniovi.es (R.F.)
2 Physics Department, University of Constantine 1, Constantine 25017, Algeria; boudjadafahima@yahoo.fr
3 MALTA-Consolider Team and Departamento de Química Física, Universidad Complutense de Madrid, E-28040 Madrid, Spain; vgbaonza@ucm.es
4 Institut Lumiere Matiere, Université Claude Bernard Lyon 1, CNRS, F-69622 Villeurbanne, France
5 Instituto de Geociencias, IGEO, CSIC-UCM, E-28040 Madrid, Spain
* email : h.chorfi@umc.edu.dz

Abstract: A clear understanding of the cohesive and mechanical properties of technological materials is of capital importance especially when applications are demanded in environments with hostile thermal, stress, and chemical conditions. Since the nature of the crystalline bonding networks is ultimately responsible for the response of the compounds to these external conditions, it is rewarding and necessary to investigate how macroscopic properties correlate with chemical interactions at an atomic level. Ionic solids constitute a crystal families currently attracting interest in a variety of areas such as electronics and solar cell industries [1–3]. To this end, computer simulations constitute a practical research route to microscopically analyze strained structures of solids since geometries optimized by minimizing the crystal energy can be accurately obtained from first-principles electronic structure calculations under different stress conditions. In this study, we performed DFT calculations to obtain the critical strength of the selected materials along their main crystallographic directions. The results are analyzed in terms of the density of chemical bonds and atomic interactions in the investigated directions of these materials. We are particularly interested in general analytical functions able to represent the behavior of different types of compounds under these stress conditions and to reproduce the critical parameters. To this end, we propose a new 3D-SEOS form that uses the critical strain as the reference state, and that can be easily used to fit both the experimental and calculated stress–strain data.

[1] G. Carlotti, D. Fioretto, G. Socino, E. Verona. **Elastic properties and pressure induced transitions of ZnO polymorphs from first-principle calculations.** J. Phys. Condens. Matter 7, 9147–9153, 1995.
[2] Li-ZhiXu, Yue-Lin Liu and Hong-Bo Zhou. **Ideal strengths, structure transitions and bonding properties of a ZnO single crystal under tension**. J. Phys. Condens. Matter **21**, 2009.
[3] Jan Wrobel, Jacek Piechota. **On the structural stability of ZnO phases.** Solid State Communications **146**, 324–329, 2008.



Graphical abstract