Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

**Enhancing mechanical properties of calcite by Mg substitutions: An ab initio study** PAVLINA ELSTNEROVA, MARTIN FRIAK, TILMANN HICKEL, HELGE OTTO FABRITIUS, LIVERIOS LYMPERAKIS, MICHAL PETROV, DIERK RAABE, JOERG NEUGEBAUER, Max Planck Institute for Iron Research, Duesseldorf, Germany, SVETOSLAV NIKOLOV, Institute of Mechanics, Bulgarian Academy of Sciences, Sofia, Bulgaria, ANDREAS ZIGLER, Central Facility for Electron Microscopy, University of Ulm, Ulm, Germany, SABINE HILD, Department of Polymer Science, Johannes Kepler University Linz, Linz, Austria — Arthropoda representing a majority of all known animal species are protected by an exoskeleton formed by their cuticle. The cuticle represents a hierarchically structured multifunctional bio-composite based on chitin and proteins. Some groups like Crustacea reinforce the load-bearing parts of their cuticle with calcite. As the calcite sometimes contains Mg it was speculated that Mg may have a stiffening impact on the mechanical properties of the cuticle. We present a theoretical parameter-free quantum-mechanical study of thermodynamic, structural and elastic properties of Mg-substituted calcite. Our results show that substituting Ca by Mg causes an almost linear decrease in the crystal volume with Mg concentration and of substituted crystals. As a consequence the calcite crystals become stiffer giving rise e.g. to substantially increased bulk moduli.

Pavlina Elstnerova
Max Planck Institute for Iron Research, Duesseldorf, Germany

Date submitted: 04 Jan 2011 Electronic form version 1.4