Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

First-principles investigation of pressure-induced amorphization in zeolites INMACULADA PERAL, JORGE INIGUEZ[1], ICMAB–CSIC — Crystalline zeolites can be transformed into amorphous structures by application of pressure, without ever forming a liquid. Upon release of the applied pressure, some zeolites transform back to their crystalline structure while others do not. Thus, zeolites are very interesting from the point of view of the theories trying to explain *reversible* amorphization by pressure [Cohen et al., JNCS 307-310, 602 (2002)]. On the other hand, recent studies of the amorphization process in zeolites have led to the identification of co-existing phases of the same composition but markedly different densities and degrees of disorder [Greaves et al., Nat. Mats. 2, 622 (2003)]. Further, it has been argued that upon application of pressure (or, equivalently, temperature) zeolites render a low-entropy, low-density, amorphous phase that could constitute a new type of glass, with physical properties that might differ considerably from those of *typical* glasses obtained by slow cooling from the melt. In this talk we will report a first-principles investigation of the structural changes induced by pressure in zeolites. More precisely, we will show results for three zeolites with the so-called LTA structure (Na-ZK4, Na-A, and an idealized SiO_2 system with the ZK4 structure). We will discuss the implications regarding the various amorphous phases experimentally found and the reversibility of the amorphization.

[1]Presenting author

Jorge Iniguez
ICMAB–CSIC

Date submitted: 15 Jan 2006 Electronic form version 1.4