Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

The effect of temperature and anisotropic pressure on the phase transitions in α-cristobalite ROMAN MARTONAK, Comenius University. SK., DAVIDE DONADIO, UC Davis, PAOLO RAITERI, MICHELE PARRINELLO, ETH Zurich, CH — The role of temperature and anisotropy of the pressure tensor in the pressure–induced transformations of α-cristobalite is investigated by means of first principle molecular dynamics combined with an improved version of the metadynamics algorithm for the study of solid-solid phase transitions[1] We reproduce for the first time the transition to $\alpha-PbO_2$ as found in experiments[2] and we observe that the transition paths are qualitatively different and yield different products whether the applied pressure is hydrostatic or not. While in hydrostatic conditions $\alpha-PbO_2$ or stishovite is obtained depending on the temperature and initial conditions, more complicated pathways with several metastable structures are followed upon non-hydrostatic compression and post-stishovite phases are obtained. Based of our simulations, we predict the metastability of a new class of high pressure polymorphs of silica obtained by non-hydrostatic compression.

[1]R. Martoňák, D. Donadio, A. R. Oganov and M. Parrinello, Nat. Mat. **5**, 623 (2006).
[2]L. S. Dubrovinsky *et al.* Chem. Phys. Lett. **333**, 264 (2001).

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Date submitted: 13 Nov 2007 Electronic form version 1.4