

Abstract Submitted  
for the MAR17 Meeting of  
The American Physical Society

**Reaction profiles and energy surfaces of compressed species under extreme conditions**<sup>1</sup> NOHAM WEINBERG, University of the Fraser Valley, JACOB SPOONER, Simon Fraser University, BRANDON YANCIW, BRANDON SMITH, University of the Fraser Valley — Both experiment and first principles calculations unequivocally indicate that properties of elements and their compounds undergo a tremendous transformation at ultra-high pressures exceeding 1 Mbar due to the fact that the difference between intra- and intermolecular interactions disappears under such conditions. Yet, even at much milder pressures of 50-300 kbar, when molecules still retain their individual identity, their chemical properties and reactivity change dramatically. Since kinetics and mechanisms of condensed-phase reactions are described in terms of their potential energy (PES) or Gibbs energy (GES) surfaces, chemical effects of high pressure can be assessed through analysis of pressure-induced deformations of GES of solvated reaction systems. We use quantum mechanical and molecular dynamics simulations to construct GES and reaction profiles of compressed species, and analyze how topography of GES changes in response to compression. We also discuss the important role of volume profiles in assessing pressure-induced deformations and show that the high-pressure GES are well described in terms of these volume profiles and the reference zero-pressure GES.

<sup>1</sup>Support of NSERC, UFV, and WestGrid is gratefully acknowledged

Noham Weinberg  
University of the Fraser Valley and Simon Fraser University

Date submitted: 11 Nov 2016

Electronic form version 1.4