Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Compression selective solid-state chemistry ANGUANG HU, Defence Research and Development Canada — Compression selective solid-state chemistry refers to mechanically induced selective reactions of solids under thermomechanical extreme conditions. Advanced quantum solid-state chemistry simulations, based on density functional theory with localized basis functions, were performed to provide a remarkable insight into bonding pathways of high-pressure chemical reactions in all agreement with experiments. These pathways clearly demonstrate reaction mechanisms in unprecedented structural details, showing not only the chemical identity of reactive intermediates but also how atoms move along the reaction coordinate associated with a specific vibrational mode, directed by induced chemical stress occurred during bond breaking and forming. It indicates that chemical bonds in solids can break and form precisely under compression as we wish. This can be realized through strongly coupling of mechanical work to an initiation vibrational mode when all other modes can be suppressed under compression, resulting in ultrafast reactions to take place isothermally in a few femtoseconds. Thermodynamically, such reactions correspond to an entropy minimum process on an isotherm where the compression can force thermal expansion coefficient equal to zero. Combining a significantly brief reaction process with specific mode selectivity, both statistical laws and quantum uncertainty principle can be bypassed to precisely break chemical bonds, establishing fundamental principles of compression selective solid-state chemistry. Naturally this leads to understand the "alchemy" to purify, grow, and perfect certain materials such as emerging novel disruptive energetics.

Anguang Hu
Defence Research and Development Canada

Date submitted: 26 Oct 2016 Electronic form version 1.4