Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Reactivity of Noble Gases under High Pressure JORGE BOTANA, Beijing CSCR, Beijing 100193, China, XIAOLI WANG, Chinese Acad Sci, Inst Solid State Phys, Key Lab Mat Phys, Hefei 230031, China , JAKOAH BRGOCH, Univ. Houston, Dept. Chemistry, Houston, TX 77204 USA., FRANK SPERA, UC Santa Barbara, Dept. Earth Science, Santa Barbara, CA 93106 USA, MATHEW JACKSON, UC Santa Barbara, Dept. of Earth Science, Santa Barbara, CA 93106 USA, GEORG KRESSE, Univ. Vienna, Faculty of Physics, A-1090 Vienna, Austria, HAIQING LIN, Beijing CSCR, Beijing 100193, China, MAOSHENG MIAO, CSU Northridge, Department of Chemistry, Northridge, CA 91330, USA — There has been recently a trend in finding how high pressure can enable the reactivity of noble gases (NG). The discovery of Xe oxidation meant a doctrinal change, by showing that a complete electron shell is not inert to reaction. However reduced NG atoms in chemical compounds were not found, neither experimentally nor theoretically. Using first-principles electronic structure calculations coupled with a structure prediction method, we have found that Xe, Kr, and Ar can form thermodynamically stable compounds with Mg at high pressure (≥ 125, ≥ 250, and ≥ 250 GPa, respectively). The compounds are metallic and the NG atoms are negatively charged, suggesting that chemical species with a completely filled shell become reduced. Moreover, Mg_2NG are high-pressure electrides. Inspired by recent research,[1] we extended the study to the mixtures of different compounds of Mg, Li and N with He. We performed a systematic structure search from 10^{-4} to 300 GPa for mixtures with different ratios of He.

[1] arXiv:1309.3827 [cond-mat.mtrl-sci]

Jorge Botana
Beijing Computational Science Res Ctr

Date submitted: 10 Nov 2016 Electronic form version 1.4