Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Electron counting and a large family of two-dimensional semiconductors MAOSHENG MIAO, Department of Chemistry and Biochemistry, California Sate University Northridge, JORGE BOTANA, Beijing Computational Science Research Center, EVA ZUREK, Department of Chemistry, University at Buffalo, JINGYAO LIU, Institute of Theoretical Chemistry, Jilin University, WEN YANG, Beijing Computational Science Research Center — Two-dimensional semiconductors (2DSC) are currently the focus of many studies, thanks to their novel and superior transport properties that may greatly influence future electronic devices. The potential applications of 2DSCs range from low-dimensional electronics, topological insulators and vallytronics all the way to novel photolysis. However, compared with the conventional semiconductors that are comprised of main group elements and cover a large range of band gaps and lattice constants, the choice of 2D materials is very limited. In this work, we propose and demonstrate a large family of 2DSCs, all adopting the same structure and consisting of only main group elements. Using advanced density functional calculations, we demonstrate the attainability of these materials, and show that they cover a large range of lattice constants, band gaps and band edge states, making them good candidate materials for heterojunctions. This family of two dimensional materials may be instrumental in the fabrication of 2DSC devices that may rival the currently employed 3D semiconductors.

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Date submitted: 06 Nov 2015 Electronic form version 1.4