Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

New Monolayered Materials Exhibiting Unusual Electronic Properties[1] ALEJANDRO LOPEZ-BEZANILLA, IVAR MARTIN, Argonne Natl Lab, PETER B. LITTLEWOOD, Argonne Natl Lab James Franck Institute, University of Chicago — Computationally based approaches are allowing to progress in the discovery and design of nano-scaled materials. Here we propose a series of new mono-layered compounds with exotic properties. By means of density functional theory calculations we demonstrate that the pentagonal arrangement of SiC2 yields an inverted distribution of the p-bands which leads to an unusual electronic behaviour of the material under strain [J. Phys. Chem. C, 2015, 119 (33), pp 19469]. A different pentagonal arrangement of C atoms enables the formation of Dirac cones which, unlike graphene, exhibit a strain-mediated tunable band gap.

[1]This work is supported by DOE-BES under Contract No. DE-AC02-06CH11357

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Date submitted: 05 Nov 2015 Electronic form version 1.4