

Abstract Submitted  
for the MAR14 Meeting of  
The American Physical Society

**Outstanding mechanical properties of monolayer MoS<sub>2</sub> and its application in elastic energy storage**<sup>1</sup> QING PENG, SUVRANU DE, Rensselaer Polytechnic Institute — The structural and mechanical properties of graphene-like honeycomb monolayer structures of MoS<sub>2</sub>(g-MoS<sub>2</sub>) under various large strains are investigated using density functional theory (DFT). g-MoS<sub>2</sub> is mechanically stable and can sustain extra large strains: the ultimate strains are 0.24, 0.37, and 0.26 for armchair, zigzag, and biaxial deformation, respectively. The in-plane stiffness is as high as 120 N/m (184 GPa equivalently). The third, fourth, and fifth order elastic constants are indispensable for accurate modeling of the mechanical properties under strains larger than 0.04, 0.07, and 0.13 respectively. The second order elastic constants, including in-plane stiffness, are predicted to monotonically increase with pressure while the Poisson ratio monotonically decreases with increasing pressure. With the prominent mechanical properties including large ultimate strains and in-plane stiffness, g-MoS<sub>2</sub> is a promising candidate of elastic energy storage for clean energy. It possesses a theoretical energy storage capacity as high as 8.8 MJ/L and 1.7 MJ/kg, or 476 Wh/kg, larger than a Li-ion battery and is environmentally friendly.

<sup>1</sup>Financial support from the Defence Threat Reduction Agency (DTRA) Grant # BRBAA08-C-2-0130 and

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Date submitted: 15 Nov 2013

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