Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Anomalous Size Dependence of Optical Properties in Black Phosphorus Quantum Dots[1] XIANGHONG NIU, YUNHAI LI, HUABING SHU, JINLAN WANG, Southeast University — Understanding electron transitions in black phosphorus nanostructures plays a crucial role for applications in electronics and optoelectronics. In this work, by employing time-dependent density functional theory calculations, we systematically study the size-dependent electronic, optical absorption and emission properties of black phosphorus quantum dots (BPQDs). Both the electronic gap and the absorption gap follow an inversely proportional law to the diameter of BPQDs in conformity to the quantum confinement effect. In contrast, the emission gap exhibits anomalous size dependence in the range of 0.8-1.8 nm which is blue-shift with the increase of size. The anomaly, in fact, arises from the structure distortion induced by the excited state relaxation and it leads to huge Stokes shift in small BPQDs.

[1]NSFC(21525311,213730) in China

Xianghong Niu
Southeast University

Date submitted: 19 Oct 2016 Electronic form version 1.4