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**Tunable and Energetically Robust PbS Nanoplatelets for Optoelectronic Applications** HUASHAN LI, DAVID ZHITOMIRSKY, JEFFREY GROSSMAN, Massachusetts Inst of Tech-MIT — Beyond the tunable bandgaps as in CQDs, nanoplatelets (NPLs) provide unique electronic and optical properties that may overcome some of the challenges in CQD-based solar cells. Our ab-initio simulations shed light on the potential of PbS NPLs as tunable and energetically robust materials for novel optoelectronic devices. The results suggest that the broken symmetry in NPLs leads to planar wave functions and parity dependent quantum confinement effects. Compared to CQD assemblies, such pseudo-two-dimensional systems may provide stronger absorption and higher carrier mobility due to the distinct wave function distributions, large electronic couplings, and small hopping barriers. More importantly, while traps seem to be unavoidable even in slightly off-stoichiometric CQDs, both energetic and spatial traps are absent in PbS NPLs even in conditions far from charge balance, indicating an extraordinary robustness against off-stoichiometry as a result of surface homogeneity and sufficient cross-linking. Based on our findings, we propose several types of optoelectronic device architectures spanning photovoltaics and photodetectors that could take advantage of the superior properties found in NPLs. [1] Li, H. et al., Chem. Mater. 2016, 28, 1888.

Huashan Li
Massachusetts Inst of Tech-MIT

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