Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Atomistic model for excitons: Capturing Strongly Bound Excitons in Monolayer Transition-Metal Dichalcogenides[1] FRANK TSENG, Naval Research Laboratory, ERGUN SIMSEK, George Washington University, DANIEL GUNLYCKE, Naval Research Laboratory — Monolayer transition-metal dichalcogenides form a direct bandgap predicted in the visible regime making them attractive host materials for various electronic and optoelectronic applications. Due to a weak dielectric screening in these materials, strongly bound electron-hole pairs or excitons have binding energies up to at least several hundred meV's. While the conventional wisdom is to think of excitons as hydrogen-like quasi-particles, we show that the hydrogen model breaks down for these experimentally observed strongly bound, room-temperature excitons. To capture these non-hydrogen-like photo-excitations, we introduce an atomistic model for excitons that predicts both bright excitons and dark excitons, and their broken degeneracy in these two-dimensional materials. For strongly bound exciton states, the lattice potential significantly distorts the envelope wave functions, which affects predicted exciton peak energies. The combination of large binding energies and non-degeneracy of exciton states in monolayer transition metal dichalogendies may furthermore be exploited in room temperature applications where prolonged exciton lifetimes are necessary.

[1]This work has been funded by the Office of Naval Research (ONR), directly and through the Naval Research Laboratory (NRL). F.T and E.S acknowledge support from NRL through the NRC Research Associateship Program and ONR Summer Faculty Program, respectively

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Date submitted: 07 Nov 2014 Electronic form version 1.4