Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Exciton Radiative Lifetimes in Layered Transition Metal Dichalcogenides MAURIZIA PALUMMO, Department of Physics, University of California, Berkeley, CA 94720, USA, MARCO BENARDI, Department of Physics, University of Rome Tor Vergata, Italy, JEFFREY C. GROSSMAN, Department of Materials Science and Engineering, Massachusetts Institute of Technology, MA 02139, USA — Light emission in two-dimensional (2D) transition metal dichalcogenides (TMDs) changes significantly with number of layers and stacking sequence. While the electronic structure and optical absorption are well understood in 2D-TMDs, much less is known about exciton dynamics and radiative recombination. In this talk, we show first-principles calculations of intrinsic exciton radiative lifetimes at low temperature (4 K) and room temperature (300 K) in TMD monolayers with chemical formula MX2 (M=Mo,W and X=S,Se), in bilayer and bulk MoS2, and in two MX2 hetero-bilayers. Our results elucidate the time scale and microscopic origin of light emission in TMDs, which have been the subjects of recent intense investigation. We find radiative lifetimes of a few ps at low temperature and a few ns at room temperature in the monolayers, and slower radiative recombination in bulk and bilayer than in monolayer MoS2. The MoS2/WS2 and MoSe2/WSe2 hetero-bilayers exhibit long-lived (∼30 ns at room temperature) inter-layer excitons constituted by electrons localized on the Mo-based and holes on the W-based monolayer; this finding agrees with recent ultrafast spectroscopy experiments. We discuss how the radiative lifetime tunability can be employed to manipulate excitons in 2D-TMDs.

Marco Bernardi
Department of Physics, University of California, Berkeley

Date submitted: 12 Nov 2014 Electronic form version 1.4