Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

The role of collective motion in the ultrafast charge transfer in van der Waals heterostructures. HAN WANG, Rensselaer Polytechnic Institute, JUNHYEOK BANG, Spin Engineering Physics Team, Korea Basic Science Institute (KBSI), YIYANG SUN, Rensselaer Polytechnic Institute, LIANGBO LIANG, Oak Ridge National Laboratory, DAMIEN WEST, VINCENT MEUNIER, SHENGBAI ZHANG, Rensselaer Polytechnic Institute — The success of van der Waals (vdW) heterostructures made of graphene, metal dichalcogenides, and other layered materials, hinges on the understanding of charge transfer across the interface as the foundation for new device concepts and applications. In contrast to conventional heterostructures, where a strong interfacial coupling is essential to charge transfer, recent experimental findings indicate that vdW heterostructues can exhibit ultra-fast charge transfer despite the weak binding of these heterostructures. Using time-dependent density functional theory molecular dynamics, we find that the collective motion of excitons at the interface lead to plasma oscillations associated with optical excitation. Furthermore, instability of these oscillations explain the rapid charge transfer across the interface and are shown to be a general feature of vdW heterostructures provided they have a critical minimum dipole coupling. Application to the MoS2/WS2 heterostructure yields good agreement with experiment, indicating near complete charge transfer within a timescale of 100 fs.

Han Wang
Rensselaer Polytechnic Institute

Date submitted: 06 Nov 2015 Electronic form version 1.4