Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Dynamics of Electronic Excitations at Interfaces DMITRI KILIN, Chemistry and Biochemistry, North Dakota State University — Atomistic modeling of broad range of excited state dynamics and charge transfer reactions at metal-to-semiconductor interfaces,[1] supported metal clusters in aqueous environment,[2] as well as in organic-inorganic lead-halide perovskites[3] and laser crystals[4] is performed by a range of methodologies including reduced density operator method, with nonadiabatic coupling being computed on-the-fly along nuclear trajectory.[5] A solution for non-equilibrium density of electrons is used for determining the dynamics of formation of surface charge transfer states, computing surface photo-voltage, and rates of energy and charge transfer.[6] An average over long *ab initio* molecular dynamics trajectories provides inhomogeneous broadening of spectral lines.[7] A modification of this methodology helps to evaluate distribution of products in photoassisted reactions.[8] 1. Han, Y., et al. Mol. Phys., 2014. **112**(3-4): p. 474-484. 2. Huang, S., et. al, J. Phys. Chem. Lett., 2014. **5** (16): p. 2823-2829 3. Junkman, D., et al., Mater. Res. Soc. Symp. Proc., 2015. **1776**: p. DOI: 10.1557/opl.2015.782 4. Yao, G., et al., Mol. Phys., 2014. **11**3(3-4): p. 385-391 5. Kilina, S., et. al. Chem. Rev., 2015. **115**((12)): p. 592–5978 6. Jensen, S.J., et. al, J. Phys. Chem. C, 2016. **12**0(11): p. 5890-5905. 7. Vogel, D.J. et al., J. Phys. Chem. C, 2015. **11**9(50): p. 27954-27964. 8. Han, Y., et al., J. Phys. Chem. A, 2015. **119**(44): p. 10838-10848

Dmitri Kilin
Chemistry and Biochemistry, North Dakota State University

Date submitted: 14 Nov 2016 Electronic form version 1.4