Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

**Carrier-induced phonon stiffening and localization in rutile TiO2**
GRIGORY KOLESOV, SEAS, Harvard University, BORIS KOLESOV, Nikolaev Institute of Inorganic Chemistry, SB RAS and Novosibirsk State University, Novosibirsk, Russia , EFTHIMIOS KAXIRAS, Department of Physics, Harvard University
— Crystalline transition metal oxides such as $TiO_2$ possess attractive properties for many practical applications. Despite several decades of researching rutile $TiO_2$ carrier-ion interactions that account for many important properties of this material, such as carrier mobility, effective mass and photo-catalytic activity, are still the subject of controversy. Here we study carrier properties in rutile $TiO_2$ both experimentally, using Raman spectroscopy of photo-excited samples, and computationally, with the real-time time-dependent density functional theory (RT-TDDFT) quantum-classical method, which employs mean-field classical (Ehrenfest) dynamics to couple the electronic and ionic subsystems. From simulation we find that small polaron formation in rutile titania is a strongly non-adiabatic process with the characteristic time scale of about 55 fs. In both experiment and theory we observe an unexpected stiffening of the $A_{1g}$ phonon mode under UV illumination. We computationally analyze the polaron structure and explain the observed effect. The resulting form of the potential with respect to oxygen atoms and $t_{2g}$-orbitals of central Ti atom offers a possible explanation for an anomalous temperature-dependence of the Hall mobility in rutile titania.

Grigory Kolesov
SEAS, Harvard University

Date submitted: 11 Nov 2016 Electronic form version 1.4