Abstract Submitted
for the DAMOP17 Meeting of
The American Physical Society

Wavepacket dynamics in the scattering of hydrogen anions off vicinally nano-stepped metal surfaces[1] JOHN SHAW, HIMADRI CHAKRABORTY, Northwest Missouri State University, Maryville, MO, DAVID MONISMITH, Software Maintenance Group, Tinker AFB, Oklahoma, USA — We study the electron dynamics in monocrystalline Cu, Au and Pd surfaces [1] with stepped vicinal structures modeled in a Kronig-Penney scheme [2]. The unoccupied bands of the surface is resonantly excited *via* the charge transfer interaction of the surface with a moving hydrogen anion. The interaction dynamics are simulated in a quantum mechanical wavepacket propagation approach [3] that used parallel computations [4]. The survival probability of the interacting ion is calculated as well as the electron probability density at all times during the interaction. Animated videos are produced of the electron probability density which show that, when the electron is transferred to the metal, the first two image states are the most likely locations of the electron as it evolves through the superlattice. The survival probability shows peaks at those energies that produce standing waves between the steps on the surface when the electron is in the image state subbands. [1] Chulkov et al, *Surf. Sc.* 437, 330 (1999); [2] Mugarza and Ortega, *J. Phys. Cond. Matt.* 15, S3281 (2003); [3] Schmitz et al, *Phys. Rev. A* 81, 042901 (2010); [4] Monismith et al, submitted, *High Performance Distributed Computing (HPDC2017).*

[1]The work is supported by the XSEDE allocation grant for high performance computation.

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Date submitted: 27 Jan 2017 Electronic form version 1.4