Abstract Submitted for the MAR06 Meeting of The American Physical Society

Low Energy Inelastic Helium Atom Scattering from Monolayers L.W. BRUCH, Department of Physics, University of Wisconsin-Madison, F.Y. HANSEN, Department of Chemistry, Technical University of Denmark — A timedependent wave packet calculation for inelastic low energy helium atom scattering (HAS) by a physisorbed monolayer<sup>1</sup> is extended to much longer propagation times by adding an absorbing potential at large distances. This enables a treatment of transiently trapped helium atoms for He/Xe/Pt(111) and shows that the lifetimes are in the range 10-30 ps. The scattering of the wave packet is essentially complete when the propagation is terminated. Systematic trends for an experiment on a Xe/Pt(111) monolayer<sup>2</sup> are discussed. The remarkable inelastic intensity for the shear horizontal (SH) monolayer branch is predicted to be strongly enhanced for incident energies in the range 4 to 6 meV, somewhat below the 8.2 meV energy used in most of that experiment.

<sup>1</sup>L. W. Bruch and F. Y. Hansen, J. Chem. Phys. **122**, 114714 (2005) <sup>2</sup>L. W. Bruch, A. P. Graham, and J. P. Toennies, J. Chem. Phys. **112**,314 (2000)

> L. W. Bruch University of Wisconsin-Madison

Date submitted: 29 Nov 2005

Electronic form version 1.4