Abstract Submitted
for the DAMOP19 Meeting of
The American Physical Society

A Bayesian optimization approach for determining the molecule-surface scattering matrix from surface spin-echo experiments[1] JOSHUA T. CANTIN, University of British Columbia, GIL ALEXANDROWICZ, Swansea University, ROMAN V. KREMS, University of British Columbia — While ^{3}He spin-echo experiments have been extensively used to study surfaces, replacing ^{3}He atoms with molecules may allow for even greater insight into surface dynamics. In particular, the additional molecular degrees of freedom, such as rotation, can give us more tools with which to probe surfaces. However, these additional molecular degrees of freedom also complicate experimental interpretation. Indeed, for *ortho*-hydrogen, the molecule-surface scattering matrix has 81 complex-valued matrix elements that are, in general, functions of incident energy. Here, we discuss the application of our new transfer matrix-based theoretical framework to the case of *ortho*-hydrogen and our preliminary work in addressing the inverse scattering problem for molecule-surface scattering. As in the algorithm applied to the inverse scattering problem in quantum reaction dynamics [1], we use Bayesian optimization to determine the scattering matrix or class of scattering matrices that fit the experimental data. We also theoretically examine different experimental protocols to discern protocols more amenable to interpretation. [1] R. A. Vargas-Hernández, Y. Guan, D. H. Zhang, and R. V. Krems, arXiv:1711.06376.

[1]This work was funded by NSERC of Canada and the Horizon 2020 Research and Innovation Programme grant 772228.

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Date submitted: 01 Feb 2019 Electronic form version 1.4