Full-dimensional close-coupling study of rovibrationally inelastic scattering of SiO-H$_2$\textsuperscript{1} B. YANG, University of Georgia, X. WANG, Emory University, P. ZHANG, Duke University, P. C. STANCIL, University of Georgia, J. M. BOWMAN, Emory University, N. BALAKRISHNAN, University of Nevada Las Vegas, R. C. FORREY, Penn State University — Molecular collisional excitation rate coefficients are required to interpret spectra of molecular gas not in local thermodynamic equilibrium. Silicon monoxide (SiO) has been detected in a variety of astronomical sources and is of astrophysical importance. Its rovibrational level populations are perturbed by collisions with He, H and H$_2$. The corresponding collisional rate coefficients and their temperature dependence are largely unknown. Theoretical scattering calculations are the primary source of such rate coefficients. In this work a full-dimensional (6D) potential energy surface (PES) of SiO-H$_2$ was calculated using the high-level CCSD(T)-F12B method and fitted using an invariant polynomial approach in 6D. We performed the first full dimensional quantum close-coupling scattering calculations for SiO in collision with H$_2$ on the 6D PES. Pure state-to-state rotational excitation transitions from SiO($v_1=0, j_1=0-10$) are computed. For rovibrational transitions, state-to-state and total quenching cross sections and corresponding rate coefficients from several low-lying rotational levels in the first excited vibrational level of SiO are calculated for both para-H$_2$ and ortho-H$_2$ collisions.

\textsuperscript{1}Work at UGA and Emory are supported by NASA grant No. NNX12AF42G, at UNLV by NSF Grant No. PHY-1505557, and at Penn State by NSF Grant No. PHY-1503615.

Phillip Stancil
University of Georgia