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Quantum calculations of H_2–H_2 collisions: from ultracold to thermal energies[1] GOULVEN QUÉMÉNER, University of Colorado, JILA, Boulder, CO 80309, ROMAN KREMS, University of British Columbia, Vancouver, BC, V6T 1Z1, Canada, BALAKRISHNAN NADUVALATH, University of Nevada Las Vegas, Las Vegas, NV 89154 — We present quantum dynamics of rotational and vibrational energy transfer in collisions between two para-H_2 molecules over a wide range of energies spanning the ultracold limit to thermal energies. The calculations were carried out using a quantum scattering code [1] that solves the time-independent Schrödinger equation in its full-dimensionality without any angular momentum decoupling approximations. The sensitivity of the results to details of the interaction potential as well as the initial vibrational and rotational quantum numbers of the H_2 molecules is explored. Cross sections and rate coefficients for elastic and inelastic collisions from our calculations are compared with available experimental and theoretical results [2,3].
References: [1] R. V. Krems, TwoBC - quantum scattering program, University of British Columbia, Vancouver, Canada (2006); [2] G. Quéméner, N. Balakrishnan, and R. V. Krems, Phys. Rev. A **77**, 030704(R) (2008); [3] G. Quéméner and N. Balakrishnan, arXiv:0812.3866 (accepted in J. Chem. Phys.).

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