Full-dimensional quantum dynamics calculations of $\text{H}_2-\text{H}_2$ collisions\textsuperscript{1} BALAKRISHNAN NADUVALATH, University of Nevada Las Vegas, GOULVEN QUEMENER, JILA, University of Colorado, Boulder, ROBERT C. FORREY, Penn State University, Berks Campus, PHILLIP STANCIL, University of Georgia, Athens — We report quantum dynamics calculations of rotational and vibrational energy transfer in collisions between two para-$\text{H}_2$ molecules over collision energies spanning from the ultracold limit to thermal energies. Results obtained using a recent full-dimensional $\text{H}_4$ potential energy surface (PES) developed by Hinde [J. Chem. Phys. 128, 154308 (2008)] are compared with those derived from the BMKP PES [J. Chem. Phys. 116, 666 (2002)]. For vibrational relaxation of $\text{H}_2(v=1, j=0)$ by collisions with $\text{H}_2(v=0, j=0)$ as well as rotational excitations in collisions between ground state $\text{H}_2$ molecules, the PES of Hinde is found to yield results in better agreement with available experimental data. However, for highly efficient near-resonant rovibrational transitions that conserve the internal rotational angular momentum, both PESs yield similar results. In the absence of the near-resonance mechanism vibrational relaxation is driven by the anisotropy of the potential energy surface.

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