Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information

Photoexcited Ag ejection from a low-temperature He cluster: A simulation study by nonadiabatic Ehrenfest ring-polymer molecular dynamics†

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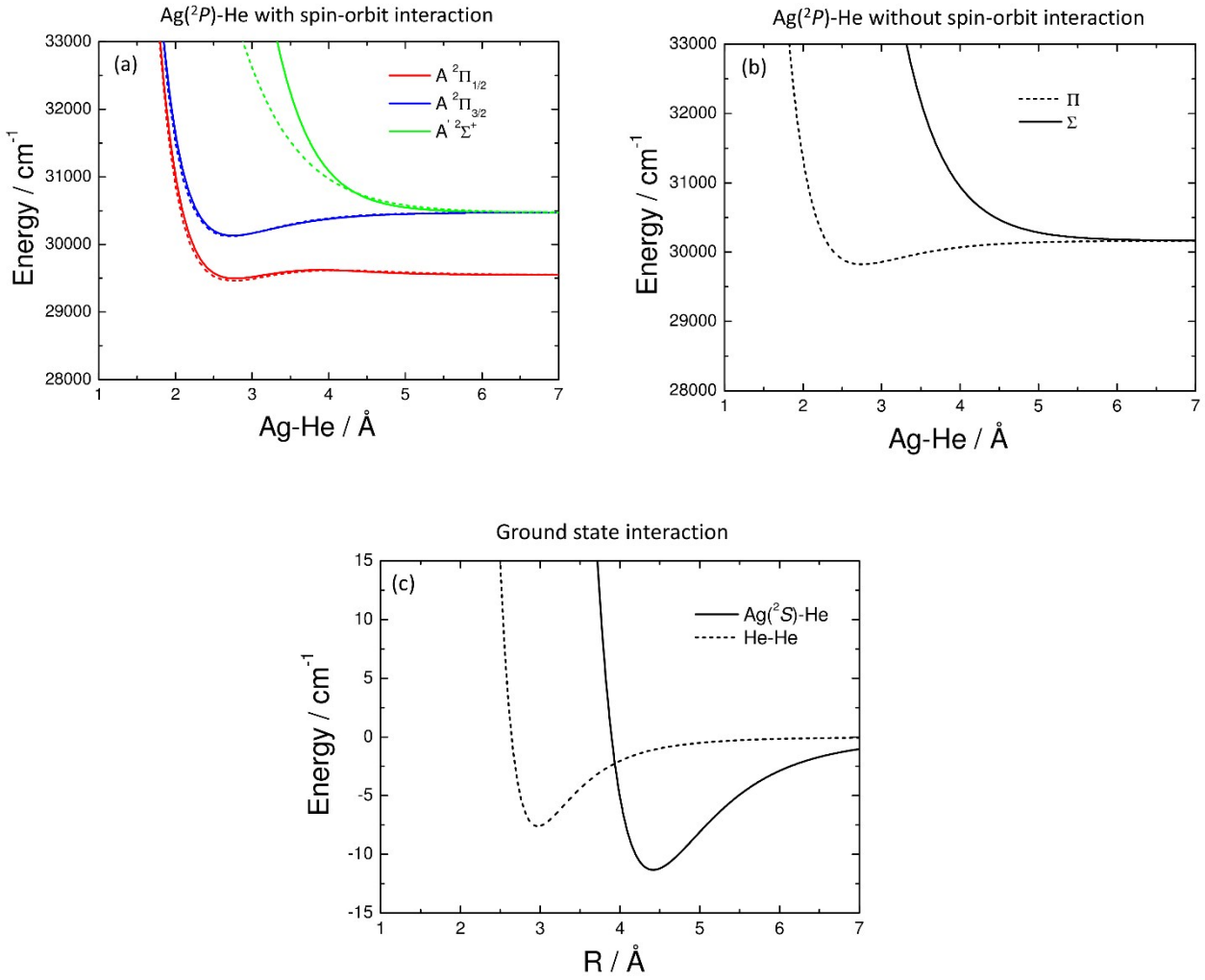

Fig. S1.

(a) and (b): Potential energy curves (solid lines) for the Ag(^{2}P)–He (with and without spin-orbit interaction) used in this work. *Ab initio* electronic structure calculation results (dashed lines) taken from the paper of Jakbek and Takami (*Chem. Phys. Lett.*, **265** (1997) 653) are also shown to demonstrate the accuracy of the potential energy functions used in this work. (c): Potential energy curves for the Ag(^{2}*S*)–He and He–He interactions.

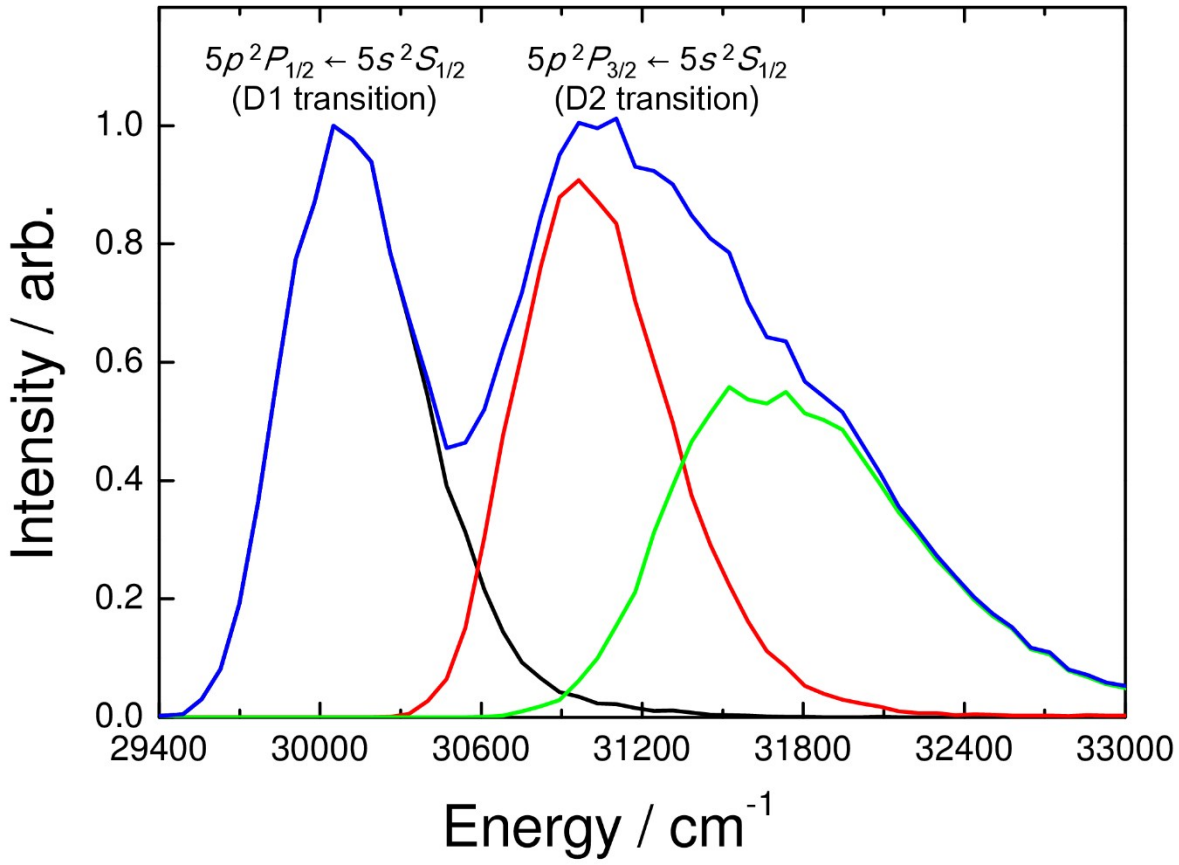

Fig. S2

Calculated total photoabsorption spectrum and decomposed spectra (contributions from the three adiabatic electronic excited states) for the $AgHe_{500}$ cluster, where atomic densities were calculated from the path-integral molecular dynamics simulations.