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A time-dependent density functional calculation of dispersion coefficients XI CHU, The University of Montana, GERRIT GROENENBOOM, University of Nijmegen, ALEX DALGARNO, Harvard University — Dispersion interactions determine the long-range potentials of approaching atoms. Long-range interactions play a critical role in elastic and inelastic scattering cross sections at low temperatures. In a buffer gas cooling experiment paramagnetic atoms are cooled to about 1 K by elastic collisions with cryogenically cooled helium-3 and trapped in a magnetic field. Anisotropic interactions can result in inelastic spin alignment changing collisions which lead to trap loss. The trapped paramagnetic atoms can be cooled further to the ultracold regime by evaporation. The efficiency of this process depends on the ratio of the rates for elastic and inelastic collisions of the paramagnetic molecules. Therefore calculating the anisotropy of the dispersion interactions is vital for predicting the success of both buffer gas cooling and evaporative cooling experiments. A time-dependent density functional approach is developed for accurate and fast determination of the scalar and tensor dynamic polarizabilites of a wide range of open shell atoms. These polarizabilites are then used to calculate the dispersion interactions between an open shell atom and a helium atom or between two open shell atoms. The results are significant in estimating the likelihood that these atoms can be trapped in a helium buffer gas and cooled by evaporation.

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