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Ab initio calculation of temperature effects in the optical response of open-shell sodium clusters[1] MARIE LOPEZ DEL PUERTO, University of Minnesota, MURILO TIAGO, JAMES CHELIKOWSKY, University of Texas at Austin — We incorporate the temperature effect on the optical absorption spectra of open-shell sodium clusters by combining pseudopotentials, Langevin molecular dynamics and time-dependent density functional theory. We have done calculations for several open-shell sodium clusters, for which experimental data is available for comparison. We find that the positions of the lower energy peaks of the calculated spectra correspond very well to the peaks in the experimental spectra. We fit the width of the peaks in the lower temperature calculations to the corresponding experimental result to obtain the instrumental line width. We then use this same width for the high temperature calculations and find very good agreement with experiment. Finally, we analyze the transitions that contribute to the observed peaks in the absorption spectra and we plot the effective valence charge density for specific transitions for each cluster.

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