AUTOIONIZING STRUCTURE IN PHOTOABSORPTION OF SMALL METALLIC CLUSTERS

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The resonance structure in photoabsorption spectra for small metal clusters and cluster ion have been studied within the many-body theory methods. The jellium model with various background charge density distributions is used to describe the positive cluster core which field the valence delocalized electrons move in. The electronic structure of ground and excited states of clusters with different number of atoms N are calculated within the Hartree-Fock (HF) approximation, and the HF wavefunctions of valence electrons are used as a basis.

The dipole-transition amplitudes, the photoionization cross sections and the oscillator strengths have been calculated with account many-electron correlations within the framework of the Random Phase Approximation with Exchange (RPAE). The well-known giant dipole resonances[1,2] in discrete spectrum are studied for clusters with different number of atoms. The very important role of continuum spectrum excitations in formation of these collective resonances has been revealed. The fragmentation of plasmon-resonance shape for the spherical clusters, for example Na_{20}, takes place due to the interaction between the resonance and single-electron modes of excitations.

The strong autoionizing structure has been found for neutral metal clusters just after the photoionization threshold, which is associated with discrete excitations of inner-shell electrons. For example, the partial 2s photoionization cross section obtained within the RPAE in spherical cluster Na_{20} ($1s^2 1p^6 1d^{10} 2s^2$) (Fig.1) demonstrates the series of 1d $\rightarrow$ np, nf autoionizing resonances with widths $\leq$ 0.02 eV. However to find this resonance structure experimentally one has to use the cooled cluster beam otherwise all this structure will be smoothed because of the thermal core oscillations.

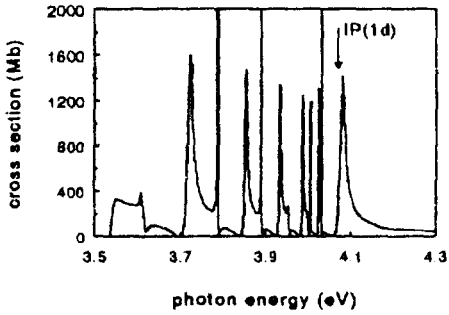

Figure 1. Photoionization cross section of Na_{20}

For negative cluster ions the collective plasmon level lies above ionization threshold and interacts with single-electron continuum spectrum. Thus, this collective resonance has a autodetachment nature and appears as a strong maximum in photodetachment cross section. In present report the giant resonances in photoabsorption spectra have been calculated for Na_9^- and Na_{19}^- negative ions and compared with other calculations[3].

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