Shape Effects in Plasmon Resonance of Sodium Clusters: A First-Principles Study

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The power computational resources, together with recent improvements in electronic structure calculation algorithms, are providing a dispensable tool for researchers in the fields of condensed matter physics. Recently, surface plasmons in metallic nanostructures have received much attention due to their novel applications in optical imaging, optical storage, ultrasensitive chemicals and biological sensing. Analyzing the sodium crystal in various shapes and sizes is of particular interest because it provides a unique way of tuning the plasmonic behavior by varying the shape and scale.

In this talk the speaker will investigate the plasmon resonances in two coupled double and quadruple atomic sodium chains as a function of interchain separation. In addition, the speaker and his group study the plasmon resonances in two coupled single-layer, double-layer, and quadruple-layers sodium 2D planes. Finally, the speaker will do the similar calculation and analysis in sodium cube and spherical cluster in body centered cubic (BCC) structure. The speaker will present a systematic study for several coupled system. In particular, the speaker will investigate the effect of size and shape of the small sodium cluster as mentioned above. The electronic ground state is treated within local density functional approximation. To compute the optical response, the group use a real-space and real-time time-dependent density functional theory code, OCTOPUS.