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Melting of Metal Clusters: A First-Principle Viewpoint

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With the rise of nanoscience the melting of finite systems has gained technical relevance. Over the last two decades experimental techniques for the accurate study of the melting of small metal clusters have been developed in several laboratories. In particular the melting of small size selected sodium [1] and aluminum [2] clusters have been studied in great detail.

In this talk I will present deMon2k [3] all-electron ab-initio Born-Oppenheimer molecular dynamics (BOMD) simulations of selected sodium [4] and aluminum clusters [5]. It will be shown that a quantitative prediction of finite system heat capacity curves from BOMD simulations is possible with the used electronic structure method. Particularities of individual clusters and cluster families are discussed in detail and compared to the available experimental results and their interpretation in the literature.

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