

## **Molecular dynamic studies of melting: to trust or not to trust?**

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MD studies of melting have evolved from qualitative to highly reliable quantitative. Nowadays, computation of a PT melting curve of a substance in many cases can be done with remarkable precision and insight into the details on the atomic and even electronic scales. However, the variety of models and approaches to treat those models, varying competence of investigators often lead to controversial data. This results in confusion and mistrust to theoretical studies of melting in general. I will provide a short overview of existing models of description of materials, methods of their treatment and computation of melting temperatures. I shall describe what are the warning signs for a suspect MD study of melting and provide a few examples of careful melting studies. The major idea of this talk is to give a crash course for distinguishing between right and wrong when it comes to computing a melting curve.