THE PHYSICS COLLOQUIUM

Thursday, 10 November 2022, 4:00 p.m.
Nijenborgh 4, Lecture Hall 5115.0317 (Schröderzaal)

From atomic interactions to the melting transition

An ab-initio study on the phase transitions of the superheavy elements Og, Cn and Fl and some insights into the melting mechanism.

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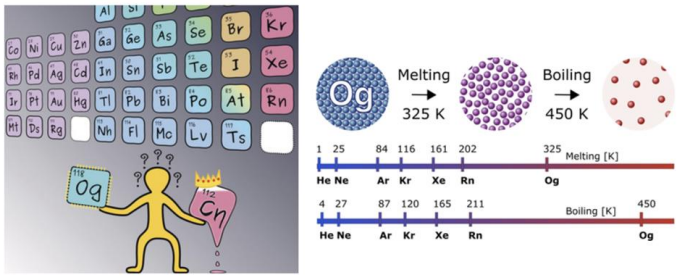
In this seminar I will present our studies on the prediction of the melting and boiling temperatures of the superheavy elements oganesson, copernicium and flerovium.

These elements do not naturally occur in the universe, but can be synthesized at various laboratories around the world. Since the nuclei of these atoms quickly decay, it is difficult to experimentally obtain knowledge on the bulk properties.



In this seminar I will explain how it is possible to obtain an estimate of the melting and boiling temperatures without any experimental input. First, the interatomic interactions were predicted based on the interaction between the electrons. Second, two numerical methods were undertaken to obtain the transition temperature: statistical sampling with Monte Carlo and first principles Thermodynamic Integration.

In the second part of my talk I will share my insights into the fundamental mechanism that drives the melting transition.

Join us for coffee starting 3:30 p.m. Refreshments will be served after the lecture.

For more information contact the host: Anastasia Borschevsky (a.borschevsky@rug.nl)
Website: http://www.rug.nl/research/vsi/colloquia/