BIO Web of Conferences **129**, 22003 (2024) https://doi.org/10.1051/bioconf/202412922003
EMC 2024

Two-dimensional few-atom noble gas clusters in a graphene sandwich

Manuel Längle[1], Kenichiro Mizohata[2], Clemens Mangler[1], Alberto Trentino[1], Kimmo Mustonen[1], E. Harriet Åhlgren[1,2], Jani Kotakoski[1]
[1]Faculty of Physics, University of Vienna, Vienna, Austria, [2]Department of Physics, University of Helsinki, Helsinki, Finland

Background incl. aims
Van der Waals atomic solids of noble gases on metals at cryogenic temperatures were the first experimental examples of two-dimensional systems [1]. Recently, such structures have also been created on surfaces under encapsulation by graphene, allowing studies at elevated temperatures through scanning tunneling microscopy [2,3]. However, for this technique, the encapsulation layer often obscures the arrangement of the noble gas atoms. When atoms are introduced into the van der Waals gap between the layers of suspended multilayer graphene the resulting structures can be directly observed at room temperature via transmission electron microscopy [4].

Methods
In this work low-energy ion irradiation has been used to irradiate suspended bilayers and double layers of graphene and hBN. Implantation parameters for noble gases from Ar to Xe were experimentally determined. Trapping occurred for Ar between 20 and 30 eV, for Kr between 25 and 60 eV, and for Xe between 15 and 65 eV. Irradiation can be carried out within the ultra-high vacuum system directly connected to a scanning transmission electron microscope [5] where the samples can be transported to a Nion UltraSTEM 100 microscope, capable of atomic-scale imaging and electron energy loss spectroscopy, without exposure to air.

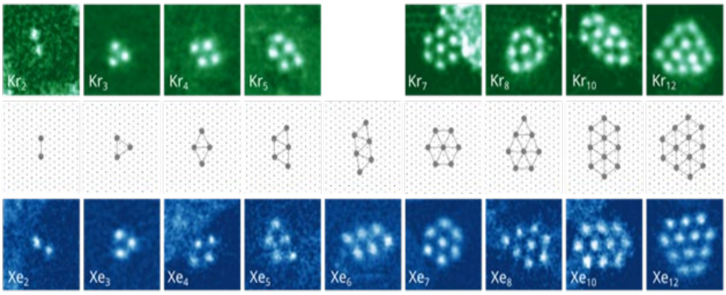
Results
The atomic structure of small Kr and Xe clusters was studied via aberration-corrected scanning transmission electron microscopy [4]. We show that small crystals ($N < 9$) arrange on the basis of the simple non-directional van der Waals interaction (Fig. 1). Larger crystals show some deviations, possibly enabled by deformations in the encapsulating graphene lattice. We further discuss the dynamics of the clusters within the graphene sandwich and show that although all the Xe clusters with up to $N \approx 100$ remain solid, Kr clusters with already $N \approx 16$ turn occasionally fluid under our experimental conditions (under a pressure of ~0.3 GPa).

The figure shows the structure of small clusters. Filtered STEM-ADF images of Kr (top row) and Xe (bottom row) including all the cases where the experimentally observed structures correspond to that with the lowest energy according to the simulations for Kr (middle row) are shown.
The encapsulated clusters show dynamic behavior such as "jumps" between different positions and occasional cluster growth and shrinking. Molecular dynamics simulations were used to understand this behavior. The trapped clusters also exhibit interesting phase behavior. While all small clusters remain solid, larger clusters exhibit either solid- or liquid-like structures depending on their size, chemical element and local microscopic environment.

Conclusion
We image noble gas atoms, their cluster formation, stability and phase in two dimensions. Due to their chemical inertness, they would not condense under normal conditions, however, when trapped between two graphene sheets the atoms are forced together by the external pressure that leads to the formation of clusters [4]. This results in a simple two-dimensional van der Waals solid that can be described to a good degree simply with the Lennard Jones

potential. This opens a way for the unexplored frontier of encapsulated two-dimensional van der Waals solids with exciting possibilities for fundamental condensed-matter physics research.

Graphic:



Keywords:

graphene, hBN, noble gas, irradiation

Reference:

[1] Jortner, J. et al., J. Chem. Phys. 42, 4250–4253 (1965).
[2] Herbig, C. et a., 2D Mater. 3, 025032 (2016).
[3] Valerius, P. et al., Phys. Rev. B 96, 235410 (2017).
[4] Längle, M. et al., Nat. Mater. (2024).
[5] Mangler, C. et al., Microsc. Microanal. 28(S1):2940-2942 (2022)