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Deposition of C, C₂, CH, CH₂ and CH₃ onto graphene: structures and structural changes of graphene

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Abstract content
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Using energy minimization method the more stable structures of C₂, CH, CH₂ and CH₃ molecules and of defect-free graphene were found. For description of the interatomic potential we used Brenner interatomic potential [1], which is specifically parameterized for the carbon and hydrogencarbon systems. Then by the molecular dynamics method and using the same Brenner potential, computer modeling of deposition of C, C₂, CH, CH₂ and CH₃ particles onto defect-free graphene was carried out.
The results of computer simulations, the structures and the various structural changes of graphene caused by the deposition of carbon atoms and C₂, CH, CH₂ and CH₃ molecules are presented and discussed.

1. D.W. Brenner, O.A. Shenderova, J.A. Harrison, S.J. Stuart, B. Ni, S.B. Sinnot, J. Phys: Condens. Matter 14, 783 (2002).

Primary author: Mr STELMAKH, Vasiliy (Institute of Ion-Plasma and Laser Technologies)

Co-authors: Dr DZHURAKHALOV, Abdiravuf (Department of Mathematics and Computer Science, University of Antwerp); Dr YADGAROV, Ishmumin (Institute of Ion-Plasma and Laser Technologies)

Presenter: Mr STELMAKH, Vasiliy (Institute of Ion-Plasma and Laser Technologies)

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