Atomic and electronic structure of structurally modified graphene

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The ab-initio modeling method (*Quantum*-ESPRESSO program package) was used to demonstrate the possibility of the formation of a structural modification of graphene (M-graphene). The process of M-graphene formation from graphene sheets and added carbon atoms is simulated. The energetics of the interaction of added atoms with graphene has been studied in detail. The energy of formation of possible configurations with added atoms on a graphene sheet are calculated.
The processes of transition of these atoms from one configuration to another have been studied.

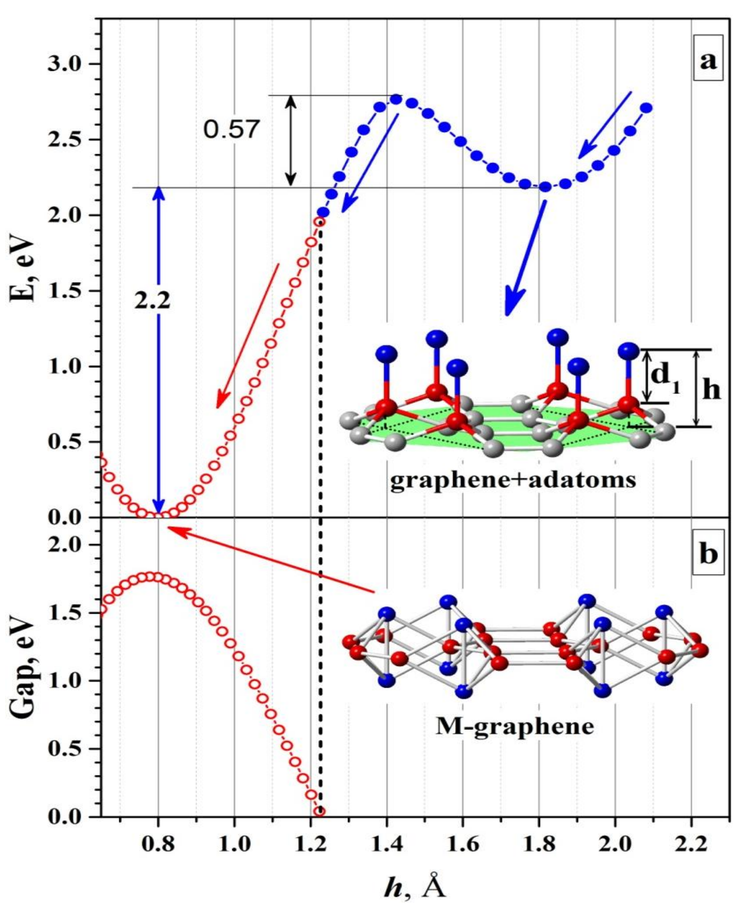

Fig.2. The scheme of M-graphene formation from the graphene and orderly located added atoms in “atom-atom” configurations

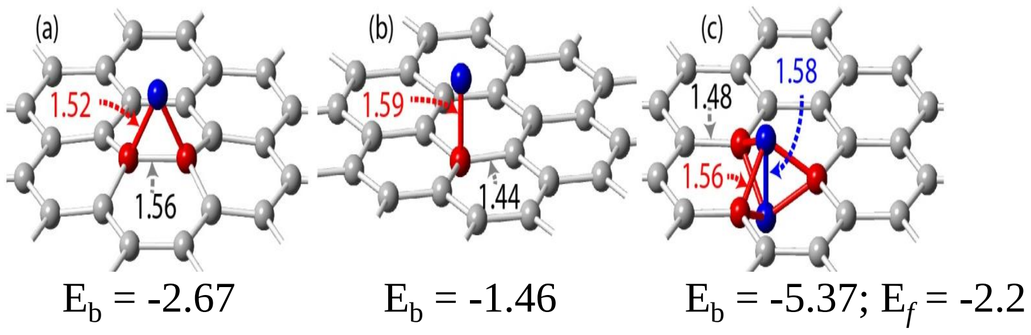

Fig. 1 Three types of the added atom configuration on a graphene sheet (eV).

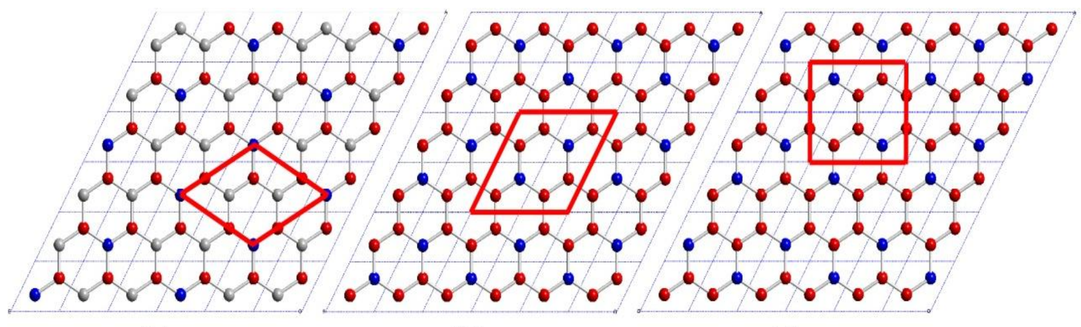

Fig. 3. Three types of the "pair" ordering on a graphene sheet.

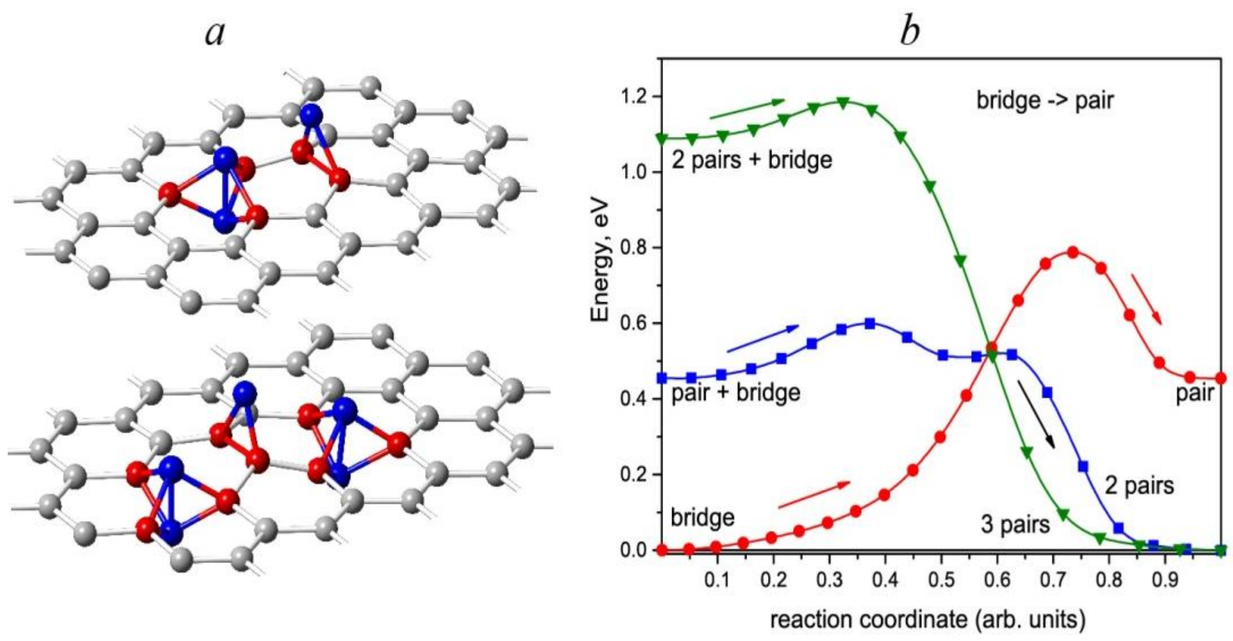

Fig.4. Change of total energy of the model structure of graphene with added atom $C_{32}C$ (4x4) as well as the force acting on an added atom, under the movement of the atom ‘form 'bridge'' to ''pair'‘ configuration and backward.

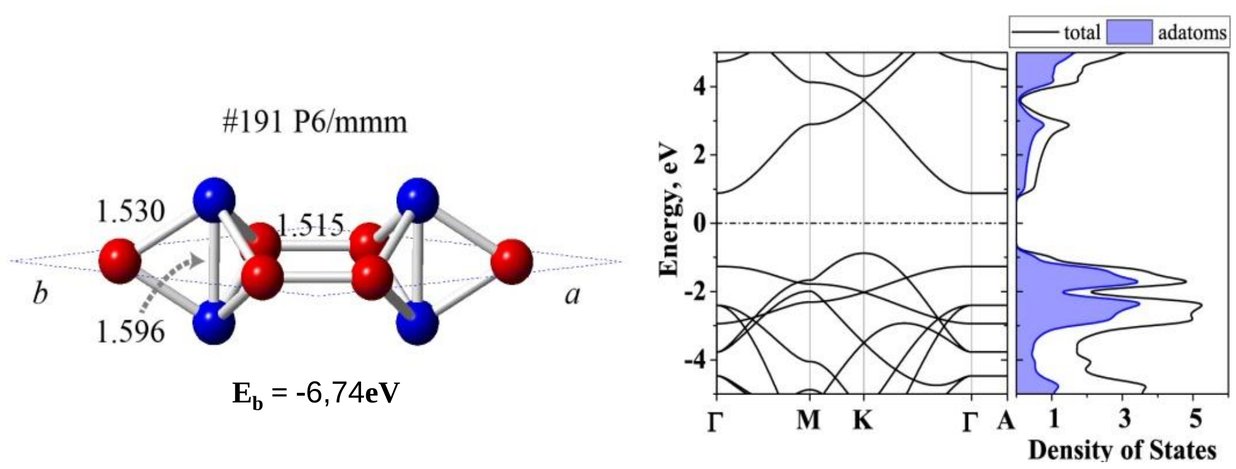

Fig.5. Unit cell and zone structure of M-graphene (Fig. 3 b)

Structural and energetic characteristics of allotropic forms of carbon

Carbon allotropes	Space-group symmetry	Number of atoms in cell	Cell parameters, Å			Gap, eV	ΔH, eV/atom
			a	*b*	*c*		
Graphene	191 P6/mmm	2	2.47	2.47	11.0	-	**-9.16**
M-graphene		10	4.89	4.89	11.0	1.76	**-8.20**
Diamond	227 Fd3m	8	3.57	3.57	3.57	4.12	**-9.02**

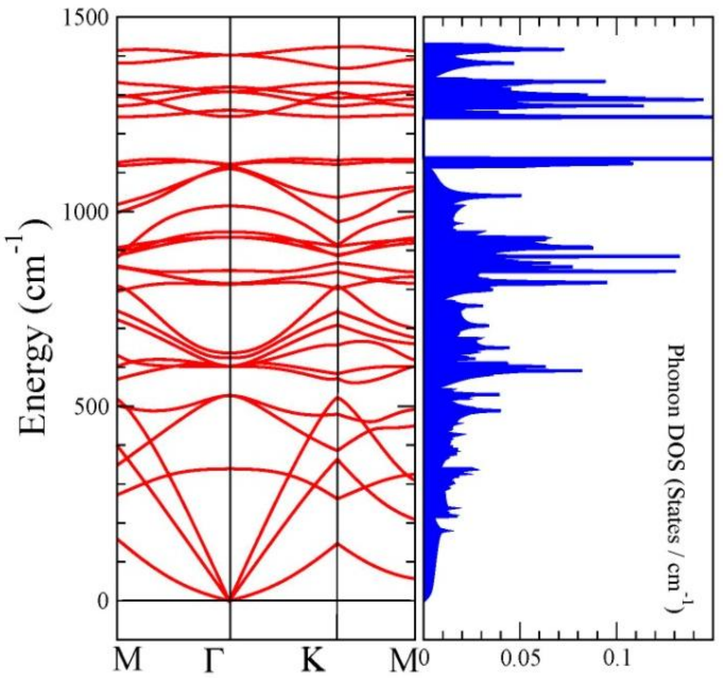

Fig.6. Phonon spectrum of M-graphene