Supplementary information for

Atomistic insights into the nucleation and growth of hexagonal boron nitride and graphene heterostructures

Mohamed Achehboune*[a], Kazem Zhour[b], Jaroslaw Dabrowski[c], Dominique Vignaud[d], Max Franck[c], Mindaugas Lukosius[c], Jean-François Colomer[a] and Luc Henrard[a]

[a]*Laboratoire de Physique du solide, Namur Institute of Structured Matter, University of Namur, Rue de Bruxelles 61, 5000, Namur, Belgium. Email : achehboune.mohamed01@gmail.com*
[b]*Institute of Physical Chemistry, University of Münster, Corrensstraße 28/30, 48149 Münster, Germany*
[c]*IHP – Leibniz-Institut für innovative Mikroelektronik, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany*
[d]*Univ. Lille, CNRS, Univ Polytechnique Hauts-de-France, UMR 8520 Institut d'Electronique de Microélectronique et de Nanotechnologie (IEMN), F-59000 Lille, France*

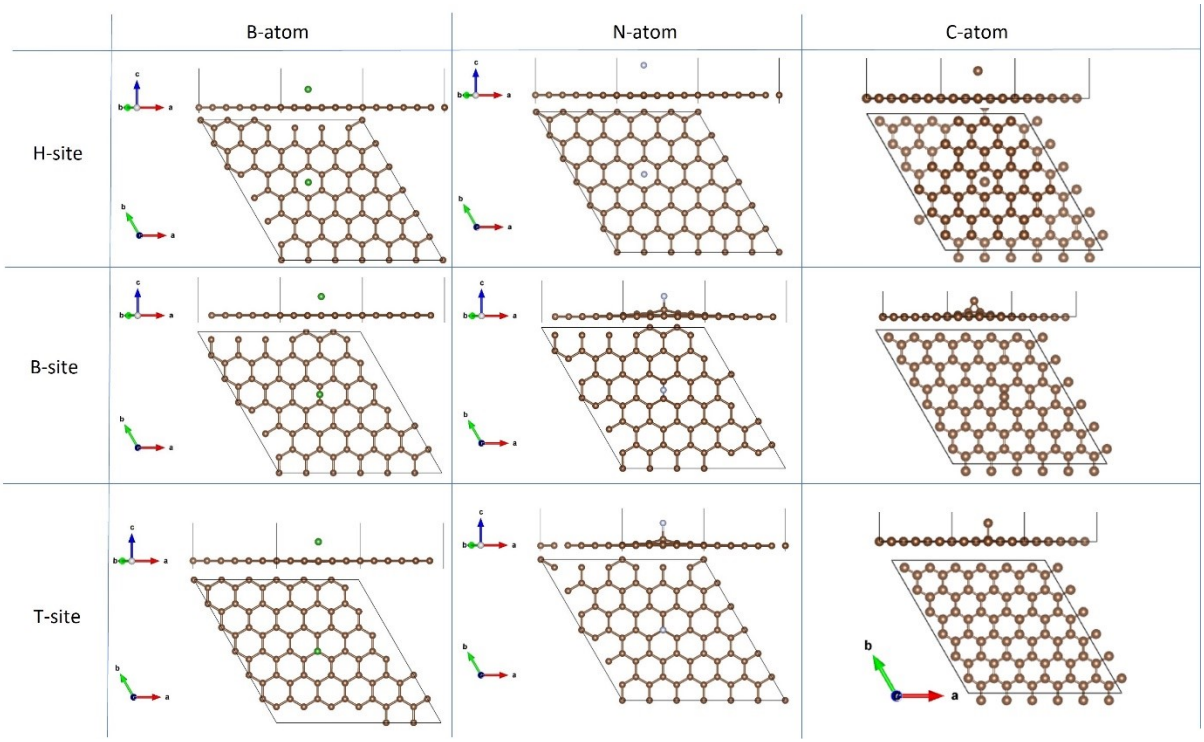

Fig. S1. *The relaxed structures for adsorbed atoms B, N and C on hBN in different positions.*

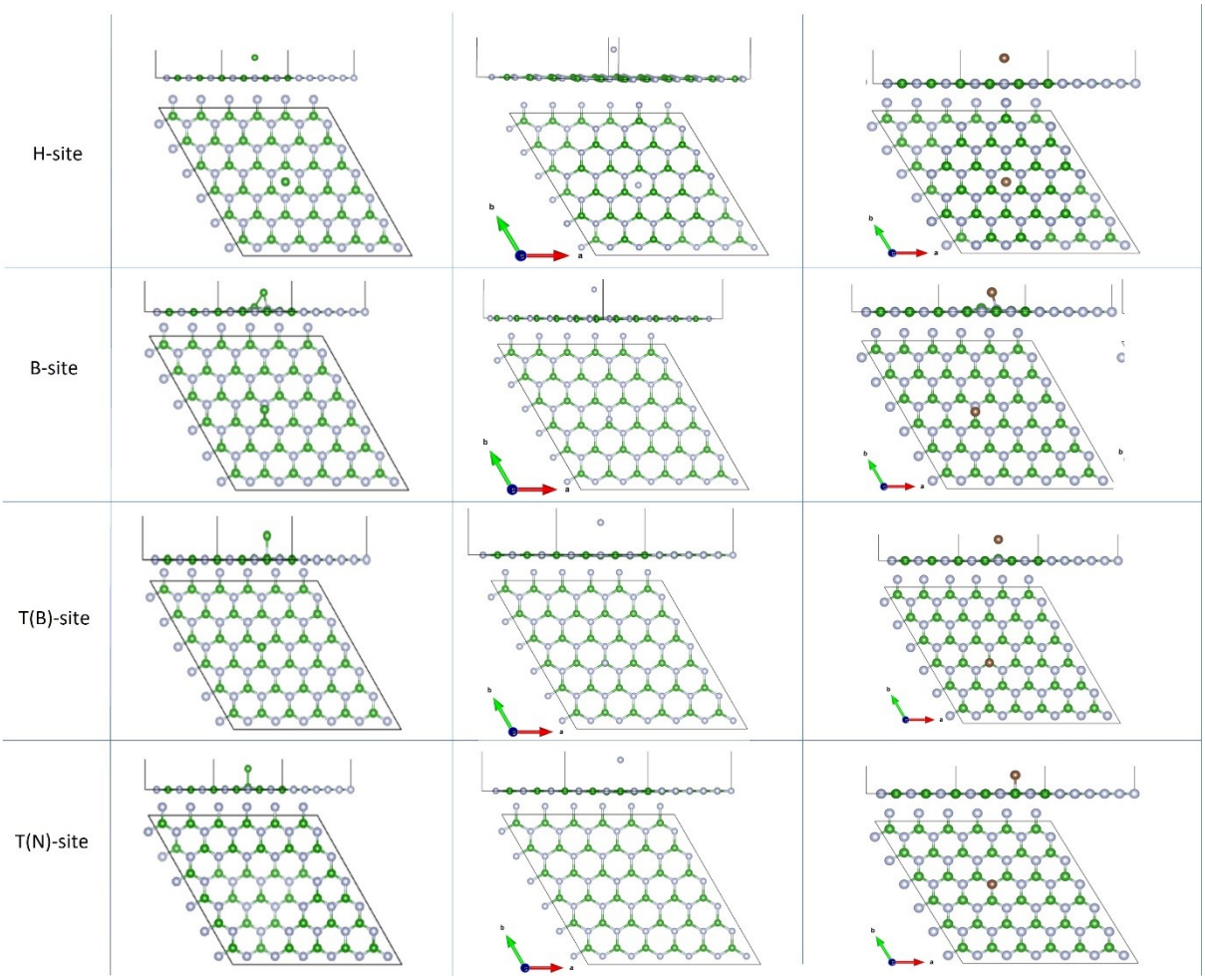

Fig. S2*. The relaxed structures for the adsorbed atoms B, N and C adsorbed on hBN in different positions.*

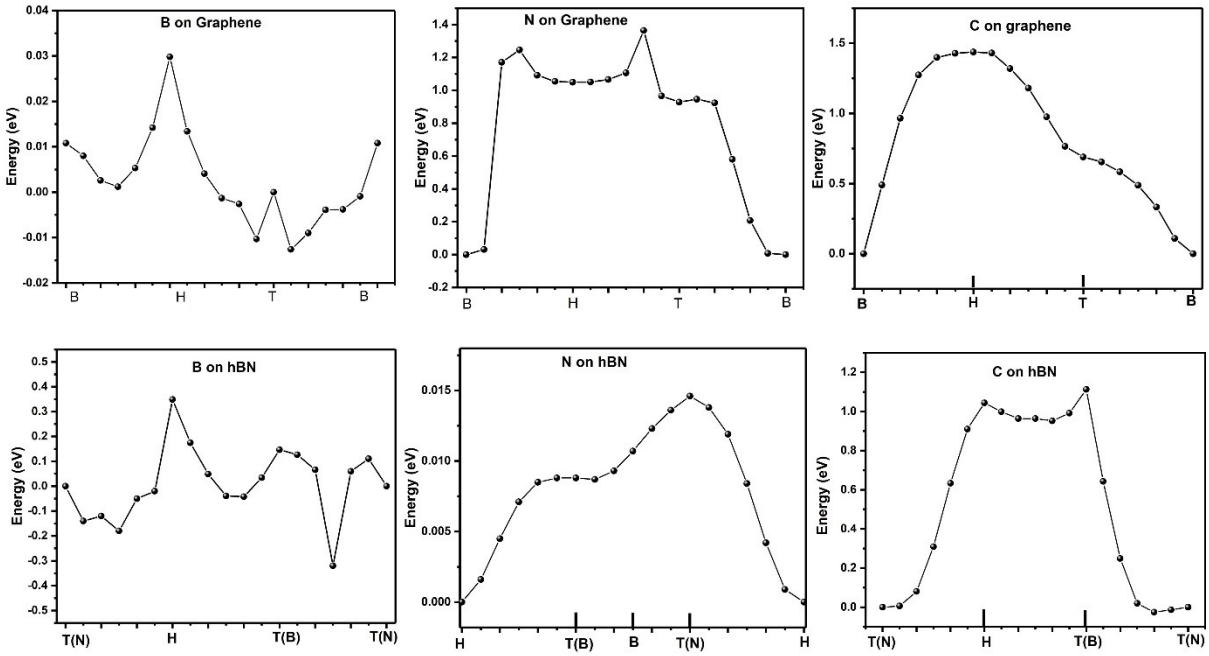

Fig. S3 *Energy barrier calculated by NEB in moving B, N and C on the graphene and hBN surfaces.*

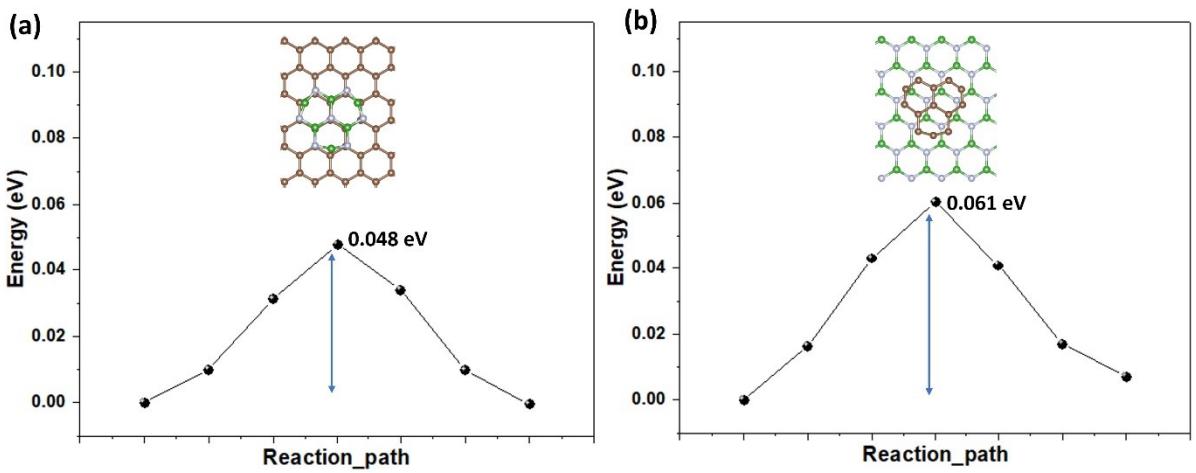

Fig. S4 *Energy barriers for (a) BN clusters on graphene and (b) Carbon clusters on hBN.*

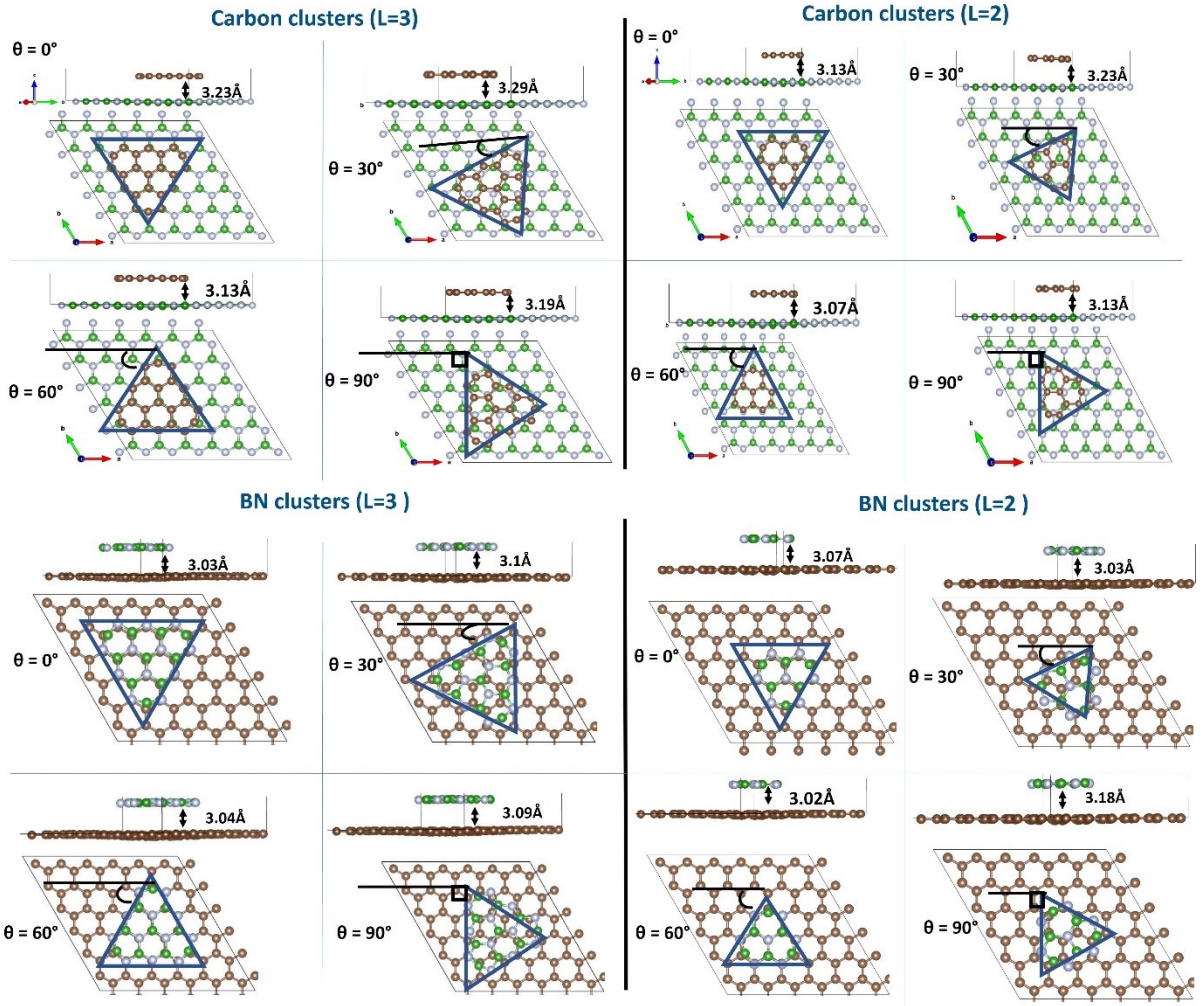

Fig. S5 *the relaxed structures of carbon and hBN clusters on graphene and hBN surfaces.*