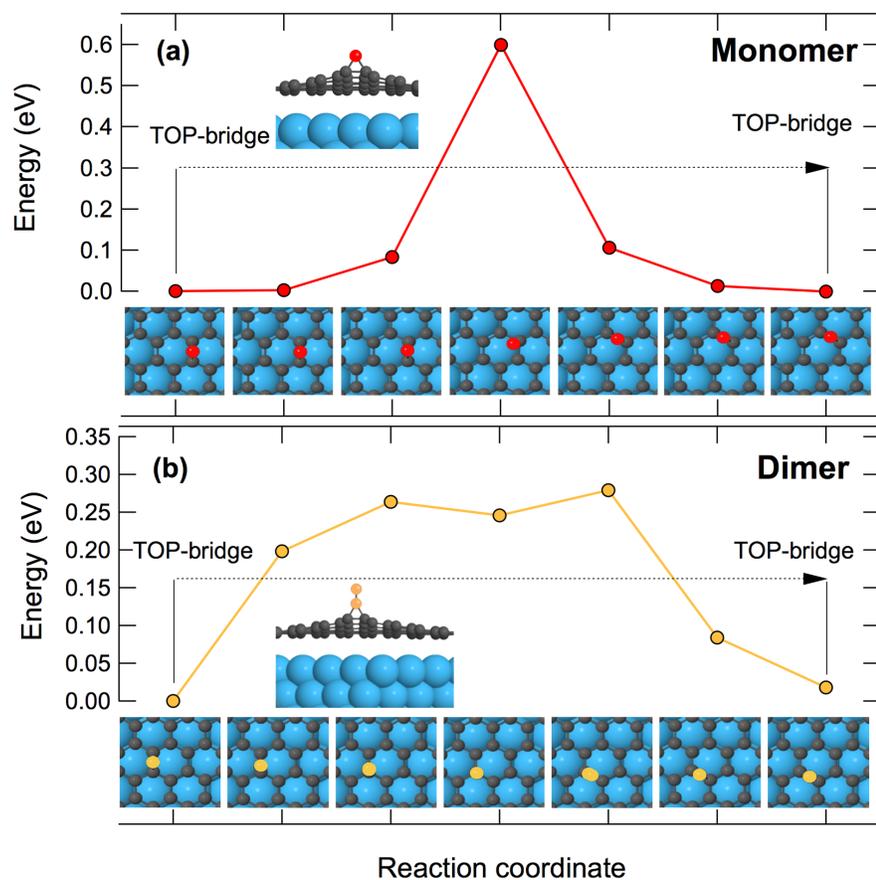


# Graphene growth by molecular beam epitaxy: an interplay between desorption, diffusion and intercalation of elemental C species on the islands

Francesco Presel,<sup>a</sup> Holly Tetlow,<sup>b</sup> Luca Bignardi,<sup>c</sup> Paolo Lacovig,<sup>c</sup> Cristian A. Tache,<sup>a‡</sup> Silvano Lizzit,<sup>c</sup> Lev Kantorovich,<sup>b</sup> and Alessandro Baraldi<sup>\*acd</sup>

## 1 Theoretical results



**Fig. S1** Calculated pathway for (a) C<sub>1</sub> and (b) C<sub>2</sub> species diffusion between adjacent unit cells on Gr supported on Ir(111). The energy variation of each system is plotted as a function of the reaction coordinate; the intermediate steps of the process are shown below.

Figure S1 shows the NEB calculations of the diffusion barriers of C<sub>1</sub> and C<sub>2</sub> species on Gr/Ir(111), between two adjacent minimum-energy adsorption sites. The results are discussed in the main text.

<sup>a</sup> Physics Department, University of Trieste, Via Valerio 2, 34127 Trieste, Italy. Tel: +39 040 3758719; E-mail: alessandro.baraldi@elettra.eu

<sup>b</sup> Physics Department, King's College London, London, WC2R 2LS, UK.

<sup>c</sup> Elettra-Sincrotrone Trieste S.C.p.A., Strada Statale 14 Km 163.5, 34149 Trieste, Italy.

<sup>d</sup> IOM-CNR, Laboratorio TASC, AREA Science Park, S.S. 14 km 163.5, 34149 Trieste, Italy.

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‡ Present address: National Institute of Materials Physics, Atomistilor Str., No. 405A, 077125 Magurele, Romania.