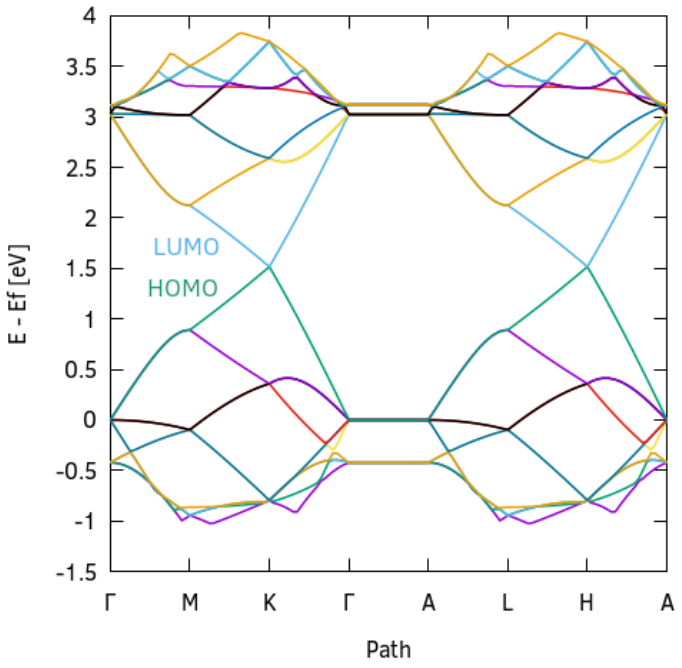
Inventory of experimental and theoretical resources available for NanoSpace COST Action	
Country:	Bulgaria
Name of Institution/Laboratory:	Bulgarian Academy of Sciences, ”E. Djakov” Institute of Electronics, Laboratory Multifunctional Materials, 72 Tzarigradsko Chausee Blvd., 1784 Sofia, Bulgaria
Contact information (name, e-mail):	Stefan Kolev Kolev; skkolev@ie.bas.bg
Website:	https://www.ie-bas.org/Departments/Multifunc.htm
Short description **(max 0.5 page)** of available techniques (experiment or theory): If appropriate, please include 1 picture/figure and caption highlighting resources.	We can employ the CP2K/Quickstep package for performing quantum mechanical calculations. The Perdew-Burke-Ernzerhof (PBE) functional is used for the implementation of the DFT method within the generalized gradient approximation (GGA). Double-zeta basis set DZVP-MOLOPT-SR-GTH can be set for all atoms in the studied systems. Dispersion interactions are accounted for by using DFT + D approach with D3 set. We can use modern calculation methods as quantum dynamics, metadynamics, TS sourcing and employing K points to simulate density of states.  Density of states of graphene calculated using 7x7x1 K points path
Sample/target description (e.g. gas, clusters, solid,…):	We can perform calculations on either gas phase, clusters or solid state systems with equal success.
How to access to experimental/computational resources (e.g. through collaboration, user facility	Our group has access to the supercomputer facility “Avitohol” of the Bulgarian Academy of Sciences.

proposal calls,….):	
References **(max 5)**:	1. S. K. Kolev, H. A. Aleksandrov, V. A. Atanasov, V. N. Popov, T. I. Milenov; Surface chemistry of reduced graphene oxide: H-atom transfer reactions; Applied Surface Science 567, 150815, 2021, IF = 6.707, (Elsevier, Netherlands), Scopus Q1, WoS Q1, SJR 1.295. 2. S. K. Kolev, H. A. Aleksandrov, V. A. Atanasov, V. N. Popov, T. I. Milenov, Interaction of Graphene with Out-of-Plane Aromatic Hydrocarbons, Journal of Physical Chemistry C 123 (35), 21448-2145, 2019, IF = 4.189, (ACS, USA), Scopus Q1, WoS Q2, SJR 1.477 3. S. K. Kolev, V. Atanasov, H. Aleksandrov, T. Milenov. Band gap modulation of graphene on SiC. Eur. Phys. J. B, 91, 272 (2018), IF:1.536, (Springer, Germany), Scopus Q2, WoS Q3, SJR 0.469 4. S. K. Kolev, P. St. Petkov, M. Rangelov, D. Trifonov, T. Milenov, G. Vayssilov. Interaction of Na+, K+, Mg2+ and Ca2+ counter cations with RNA. Metallomics, 10, 659-678 (2018), IF:3.571, (Oxford University Press, UK), Scopus Q1, WoS Q2, SJR 1.16 5. H. Iglev, S. K. Kolev, H. Rossmadl, P. Petkov, G. Vayssilov. Hydrogen Atom Transfer from Water or Alcohols Activated by Presolvated Electrons. J. Phys. Chem. Lett., 6, 6, 2015, IF:8.539, Scopus Q1, WoS Q1, SJR 4.143