SUPPLEMENTARY INFORMATION

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1 EXPLANATIONS OF THE NON-RELAXATION CALCULATION SCENARIO

If we perform the static DFT calculations, the relaxation of the hexagonal ring must be considered because the geometry of graphene or nanodome can be impacted by the oncoming noble gases atoms. In a static model, with the decreasing of the distance between a noble gas atom and graphene/nanodome, the repulsion interaction between them will be dominant. Such an interaction will give rise to the remarkable deformation of the graphene or nanodome, and the barriers will be certainly influenced. According to this, the relaxation is absolutely essential.

In fact, the dynamic simulations (FPMD) are employed in our research. By carefully analyzing the collision processes of every systems, we bring forth three interesting conclusions:

1. The effective potential felt by the noble gases atoms depend on its velocity due to the relaxation of the graphene/nanodome layer;

2. Even though the distance between the approaching single atom and graphene/nanodome is the minimum, the deformation of the membrane can also be negligible. This is a consequence of the fact that the graphene/nanodome atoms appear to lack time to relax while interacting with the fast moving atom;

3. The relaxation of the graphene layer is very small at the turning of the single atom and that the relaxation only starts when the atom has already been reflected.

These facts mean that relaxation has no significant influence on the barrier height, and therefore we are allowed to ignore any relaxation of the graphene/nanodome layer when calculating the energy barriers for penetration of the noble gas atom.

Overall, in the dynamic simulations, the barriers calculations without relaxation is closer to the true circumstance and we choose the non-relaxation scenario accordingly.

2 ELECTRON PROPERTIES

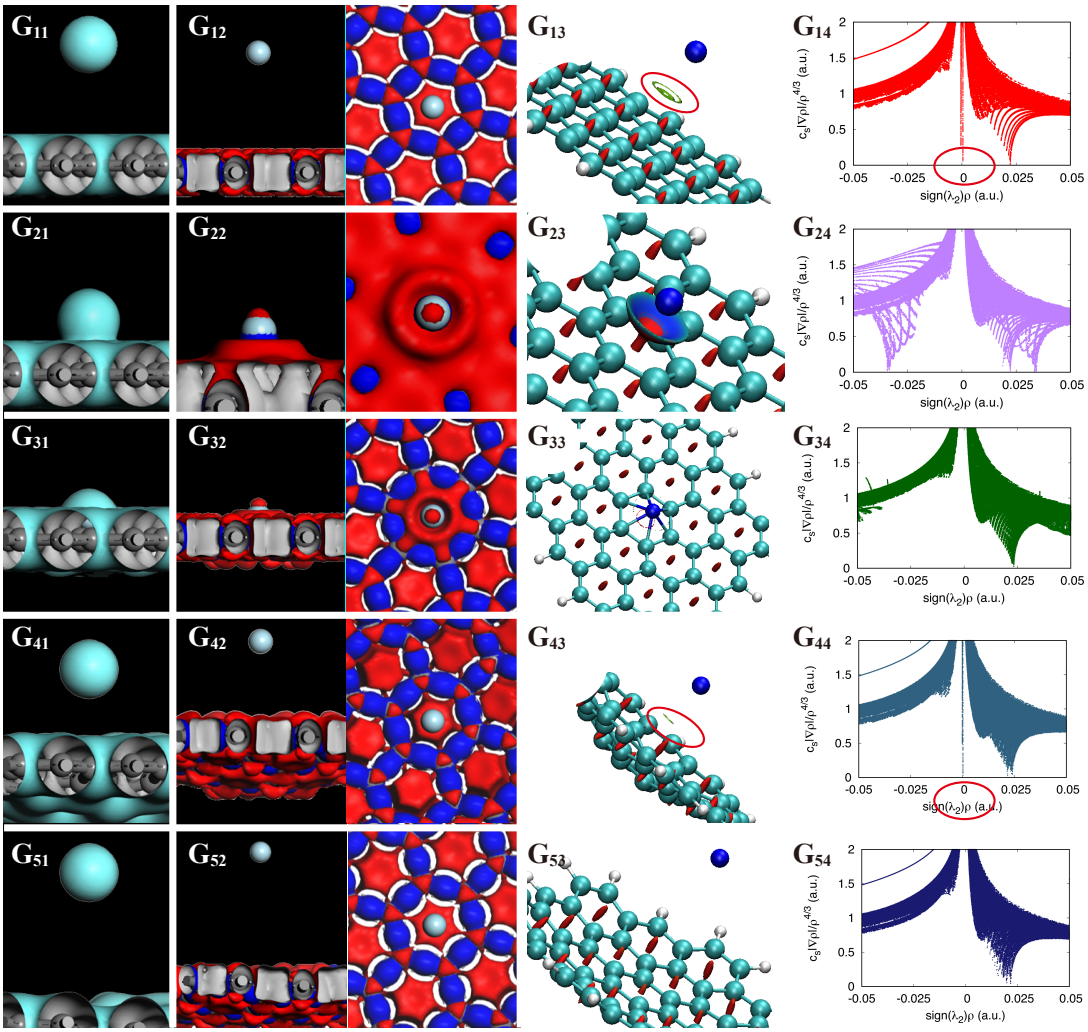

Fig. S 1: The electron related properties of the Ne-graphene collision system. D_{i1} (i=1,2,3,4,5) represents the electron density; D_{i2} (i=1,2,3,4,5) represents the deformation electron density (left: side view; right: top view); D_{i3} (i=1,2,3,4,5) represents the gradient isosurfaces of the NCI analysis. The surfaces are colored on a bulge-green-red scale according to values of the electron density multiplied by the sign of the second Hessian eigenvalue (sign$(\lambda_2)\rho$) ranging from -0.04 to 0.02 au. Blue indicates strong attractive interactions, and red indicates strong nonbonded overlap. Carbon is printed in cyan, neon in blue. D_{i4} (i=1,2,3,4,5) is the plots of the reduced density gradient versus sign$(\lambda_2)\rho$.

3 DYNAMICAL DESCRIPTION OF ATOM

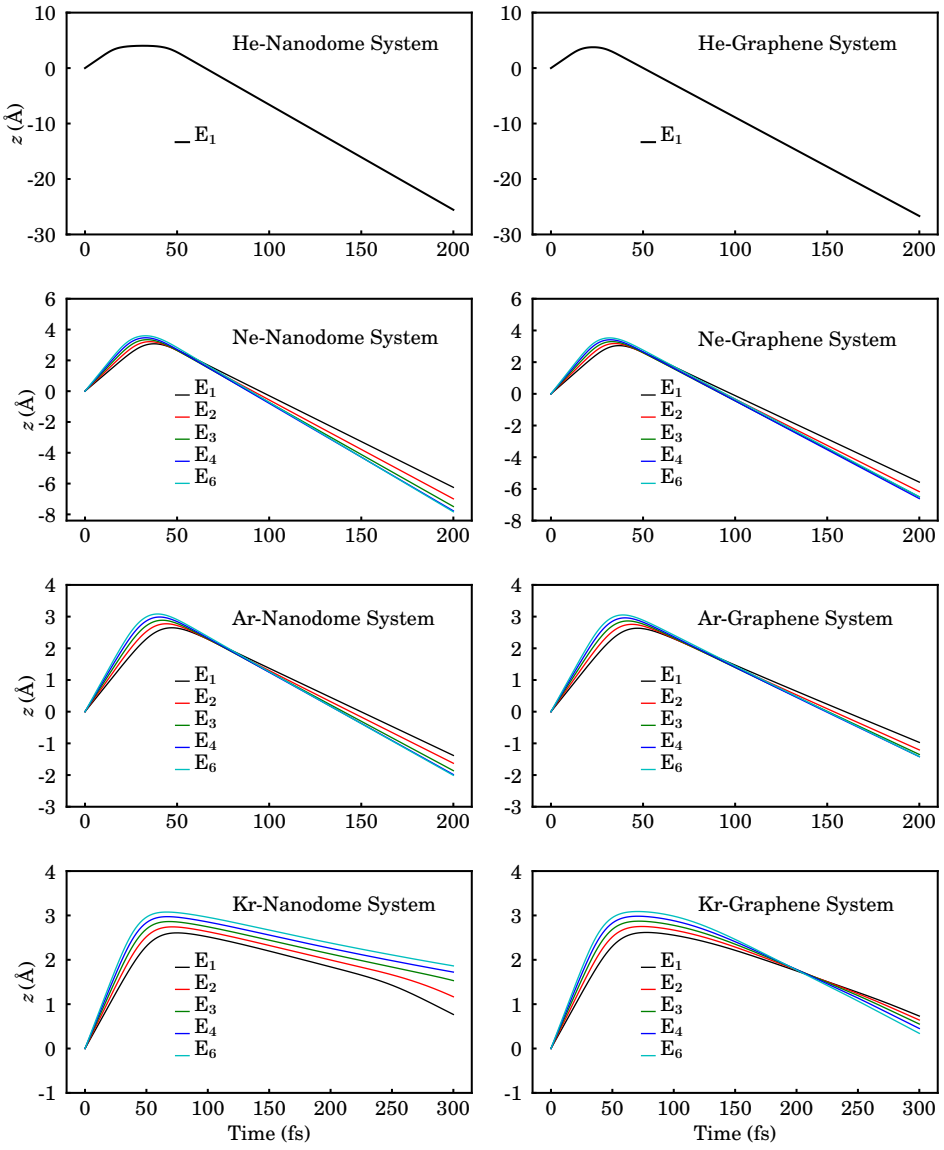

Fig. S 2: Plot of z versus t for all Atom-Structure Systems (Atom=He, Ne, Ar, Kr; Structure= Nanodome, Graphene).

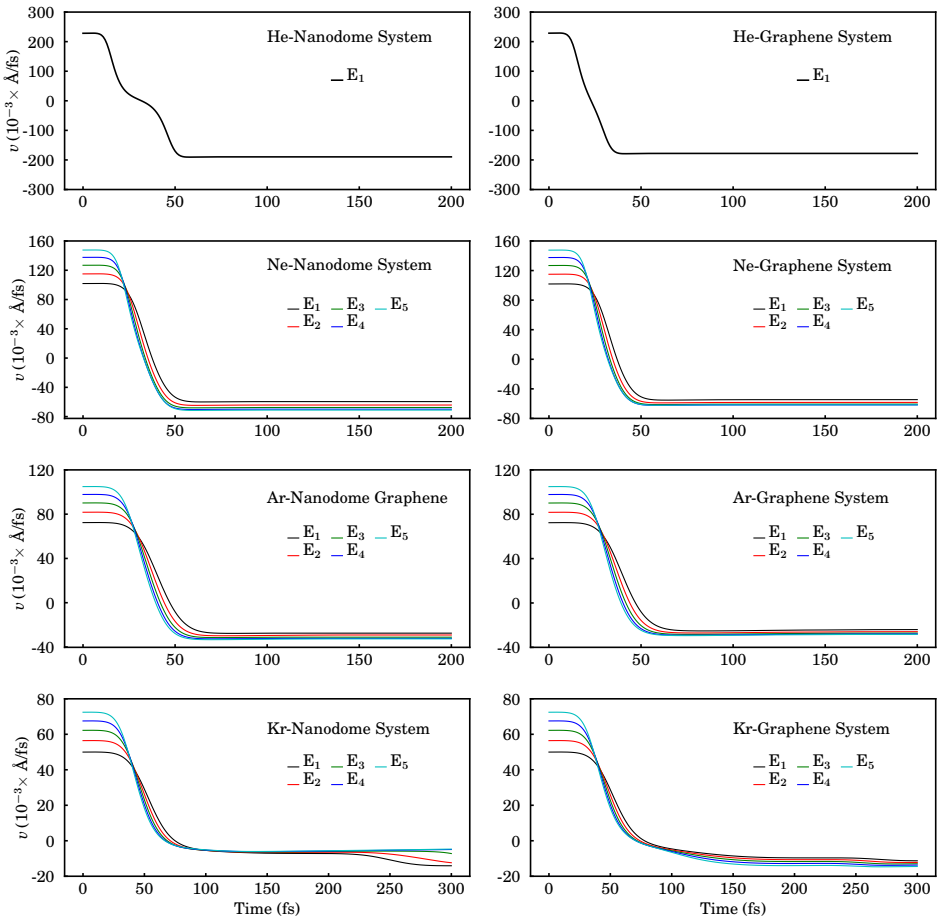

Fig. S 3: Plot of v versus t for all Atom-Structure Systems (Atom=He, Ne, Ar, Kr; Structure= Nanodome, Graphene).

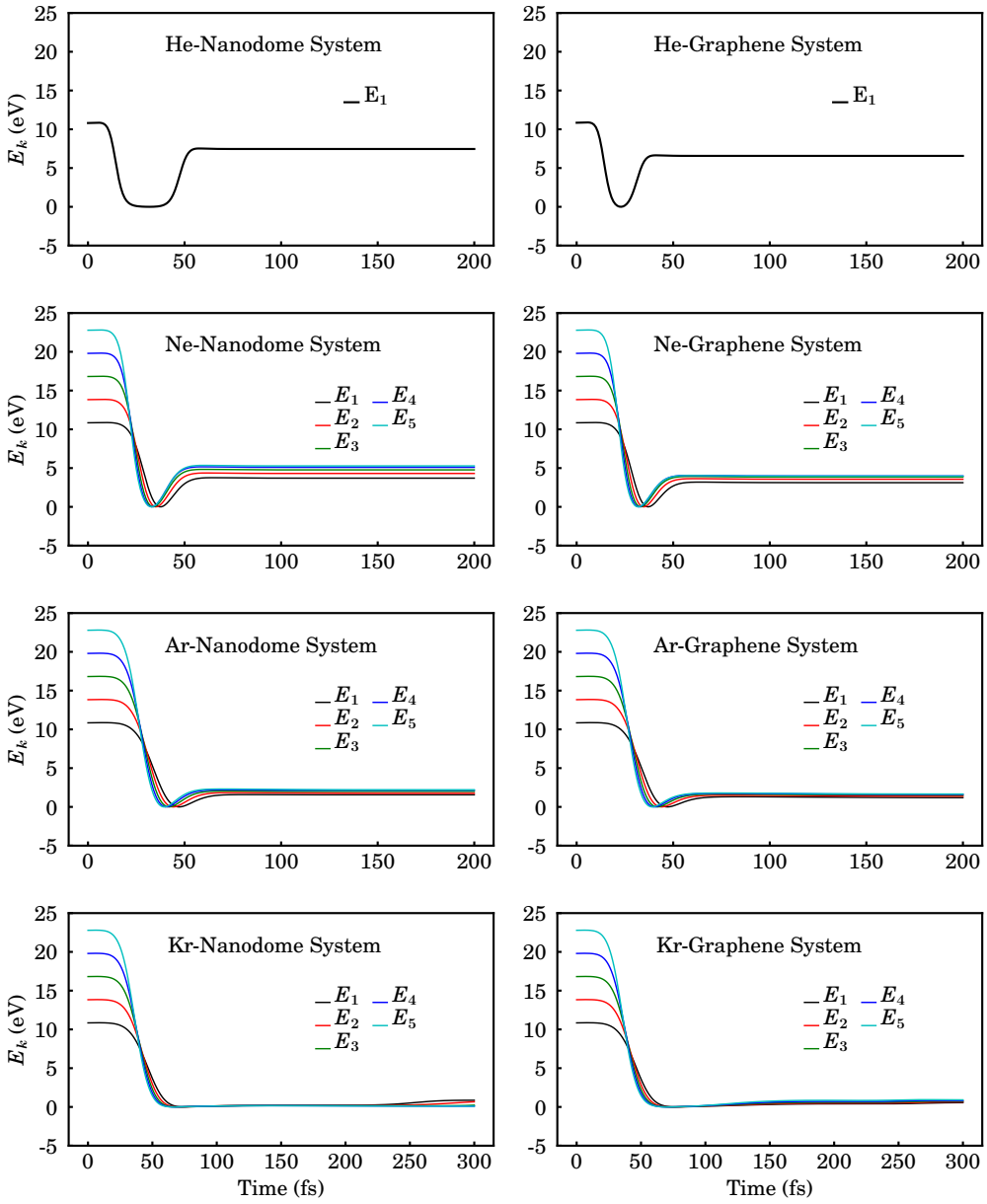

Fig. S 4: Plot of E_k versus t for all Atom-Structure Systems (Atom=He, Ne, Ar, Kr; Structure= Nanodome, Graphene).