Supplementary Materials

Ab initio Molecular Dynamics Investigation on the Permeation of Sodium and Chloride Ions through Nanopores in Graphene and hexagonal Boron Nitride Membranes

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**Reliability of Sampled Trajectories:**

The course of the fictitious kinetic energy of the electrons, ionic temperature, the Kohn-Sham, the classical, and the total (Hamiltonian) energies, during the simulations, demonstrates the stability of the calculated trajectories after an equilibration phase. These courses are presented for pure water/nanopore systems as well as for systems containing Na^+ and Cl^- in different positions.
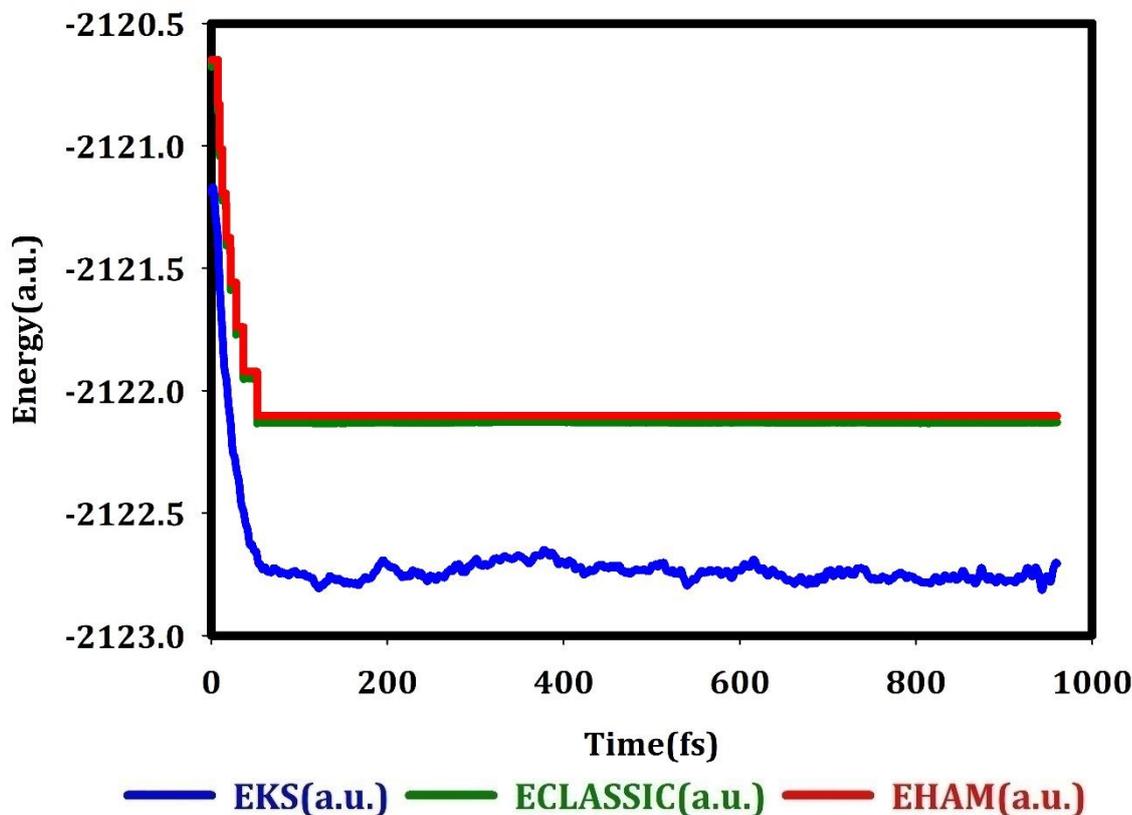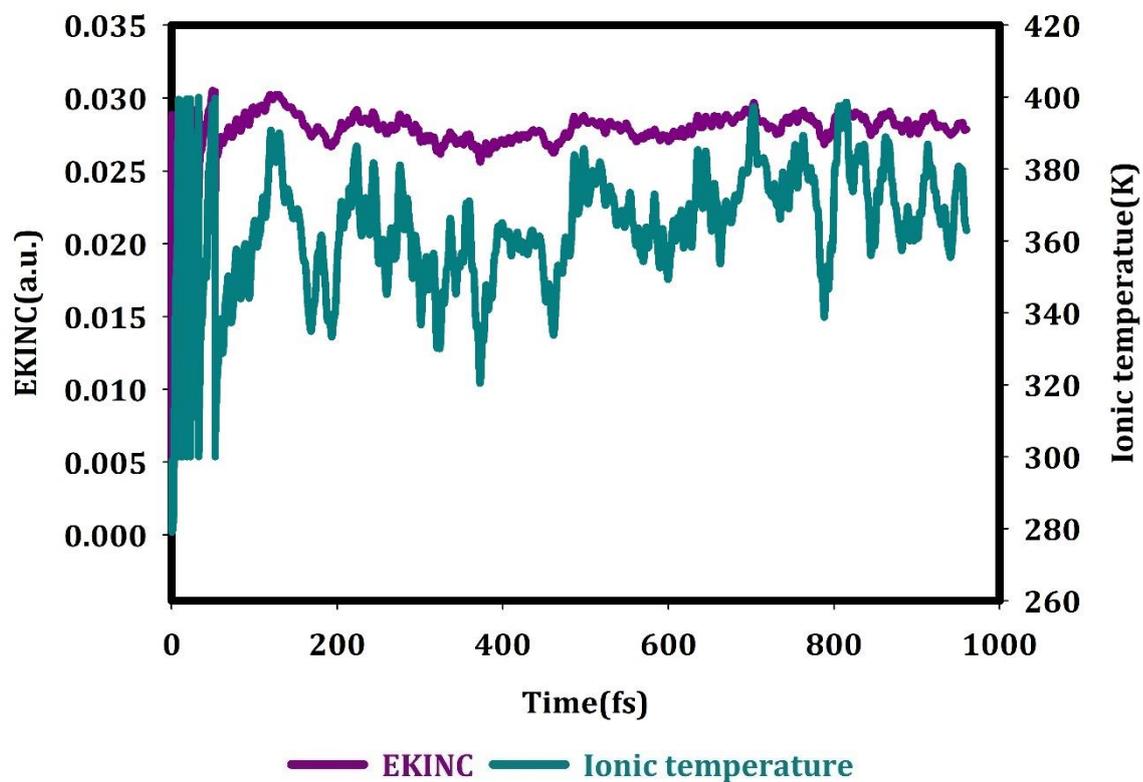

Supplementary Figure 1. Energy courses for a graphene membrane in pure water
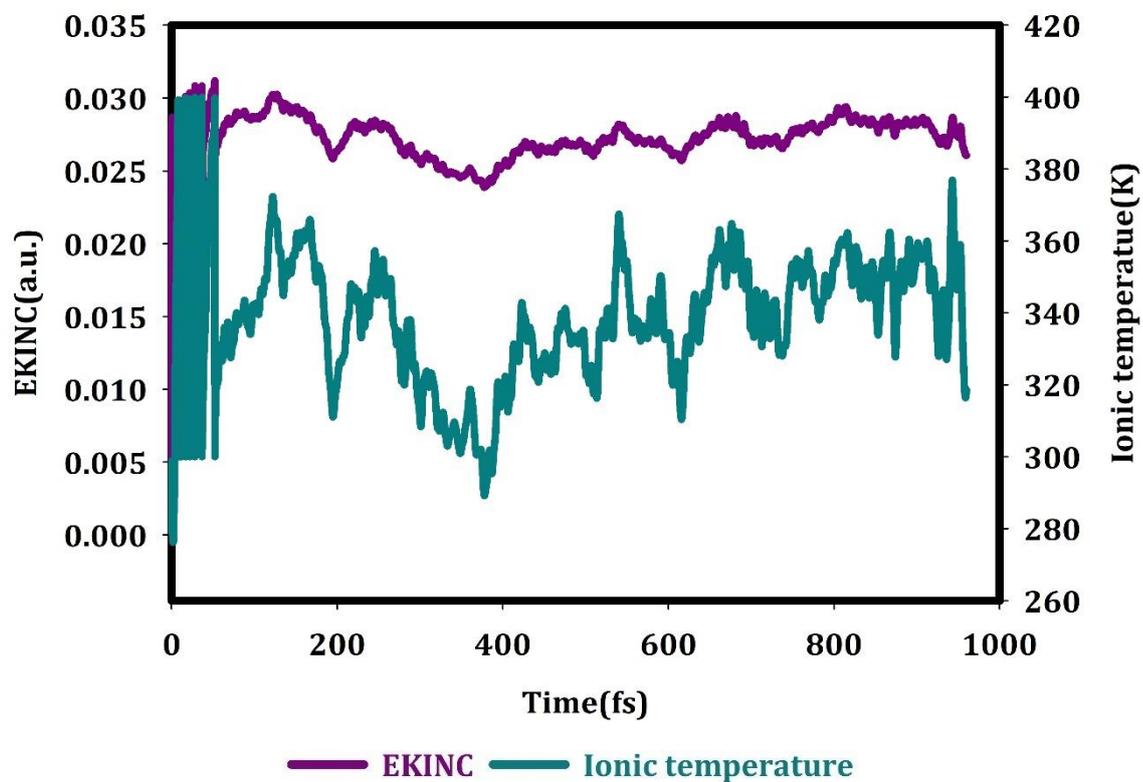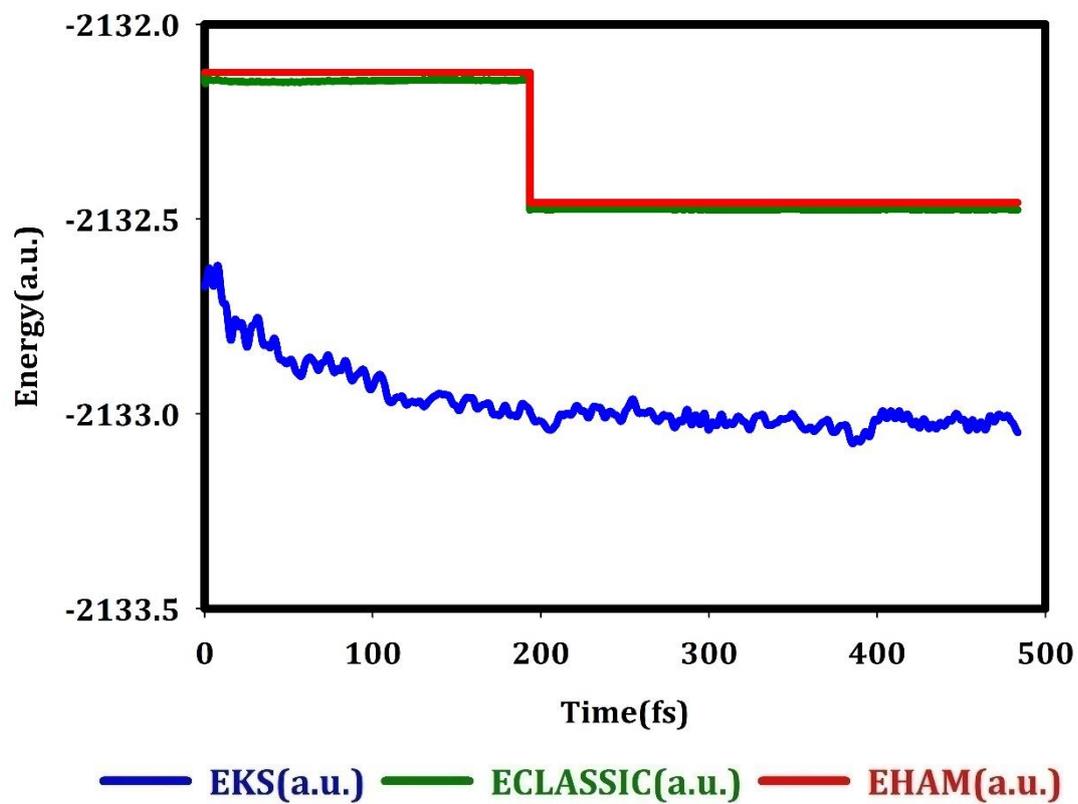
Supplementary Figure 2. The course of the fictitious kinetic energy of the electronic system and ionic temperature for a graphene membrane in pure water.
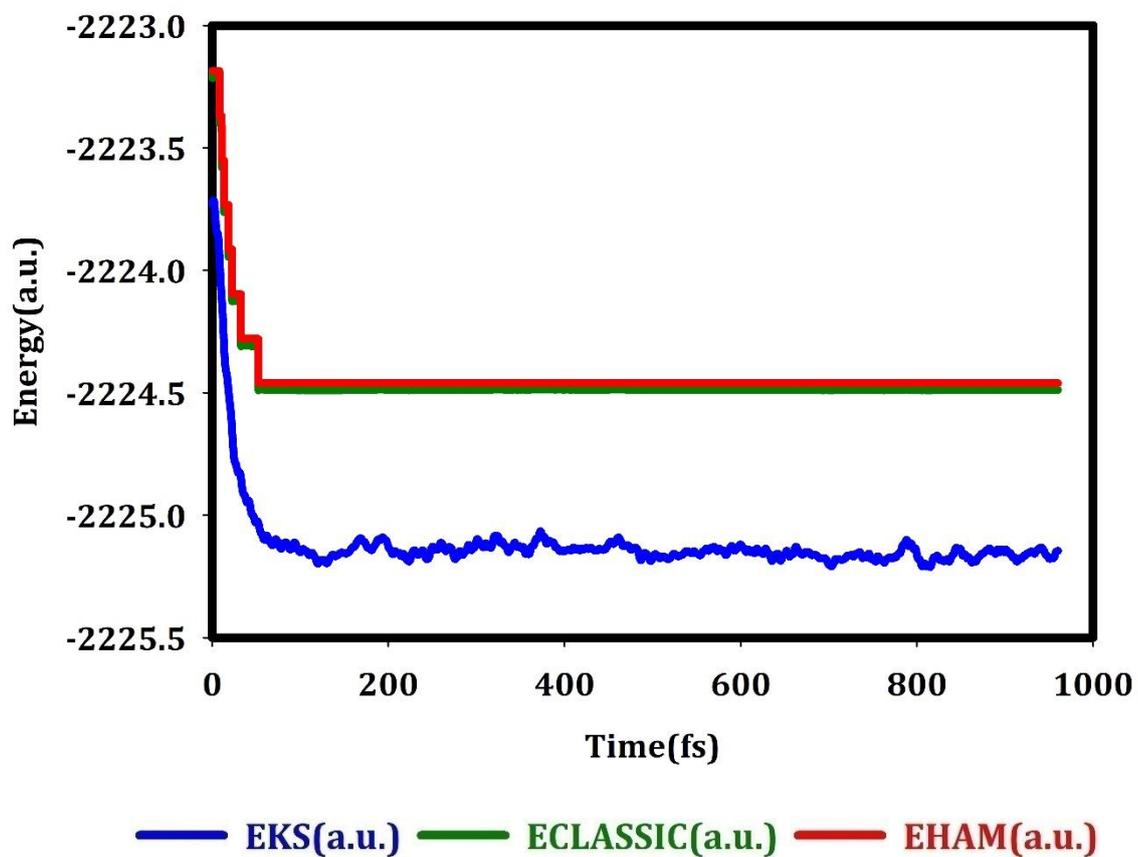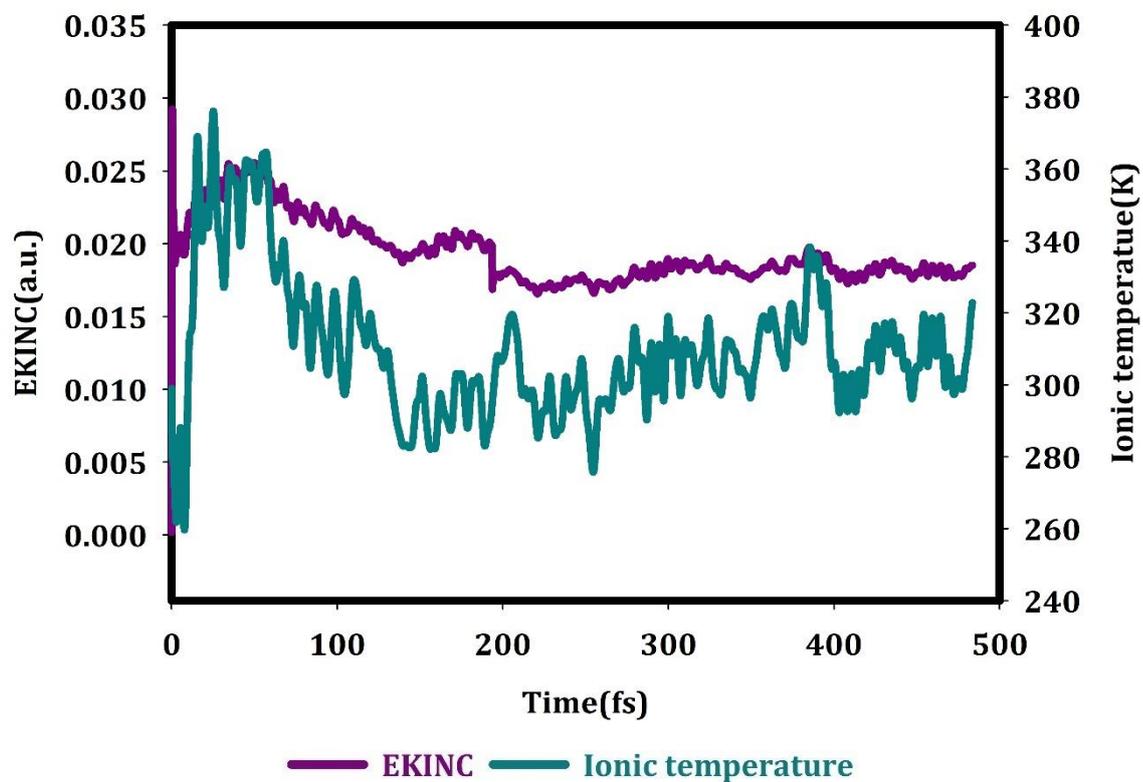
Supplementary Figure 3. Energy courses for an h-BN membrane in pure water.
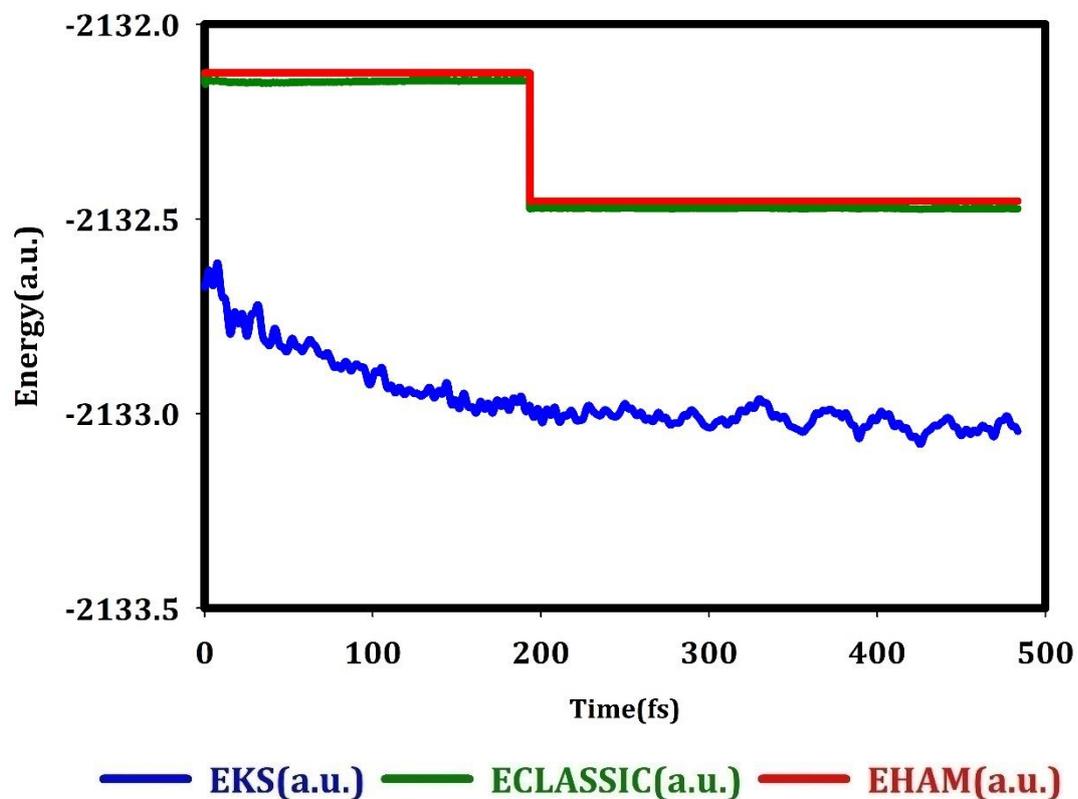
Supplementary Figure 4. The course of the fictitious kinetic energy of the electronic system and ionic temperature for an h-BN membrane in pure water.
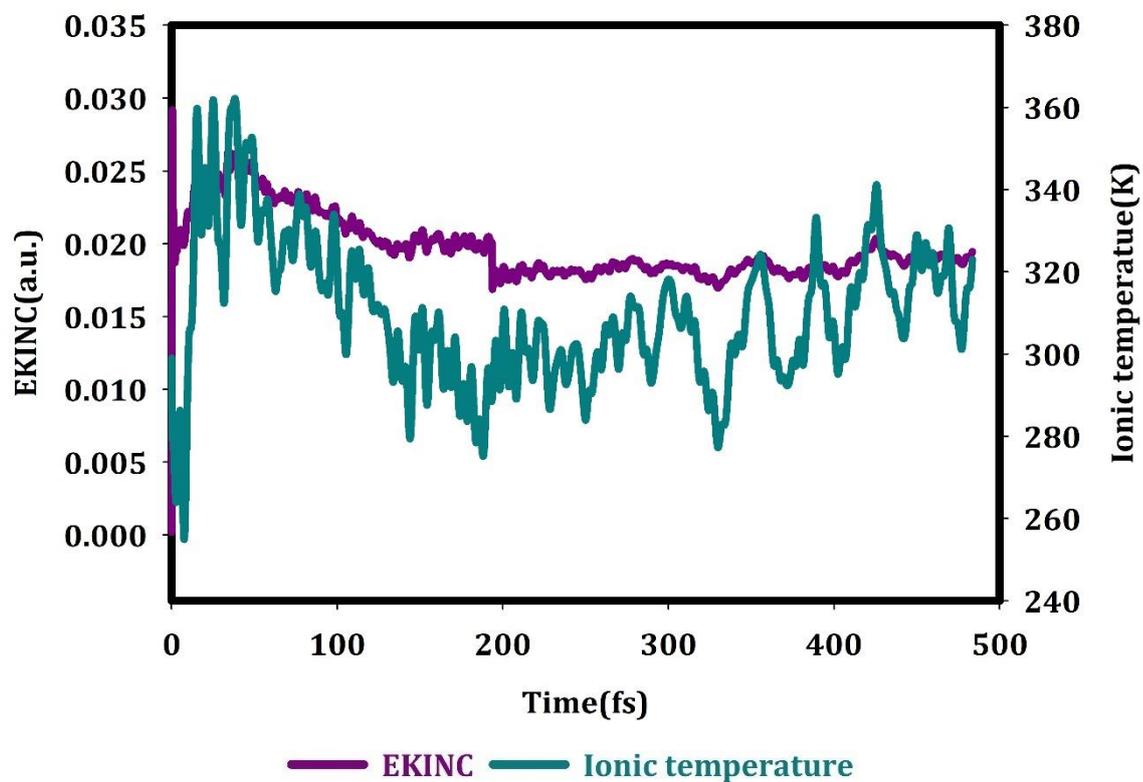
Supplementary Figure 5. Energy courses for Na^+ positioning in the center of the graphene nanopore.
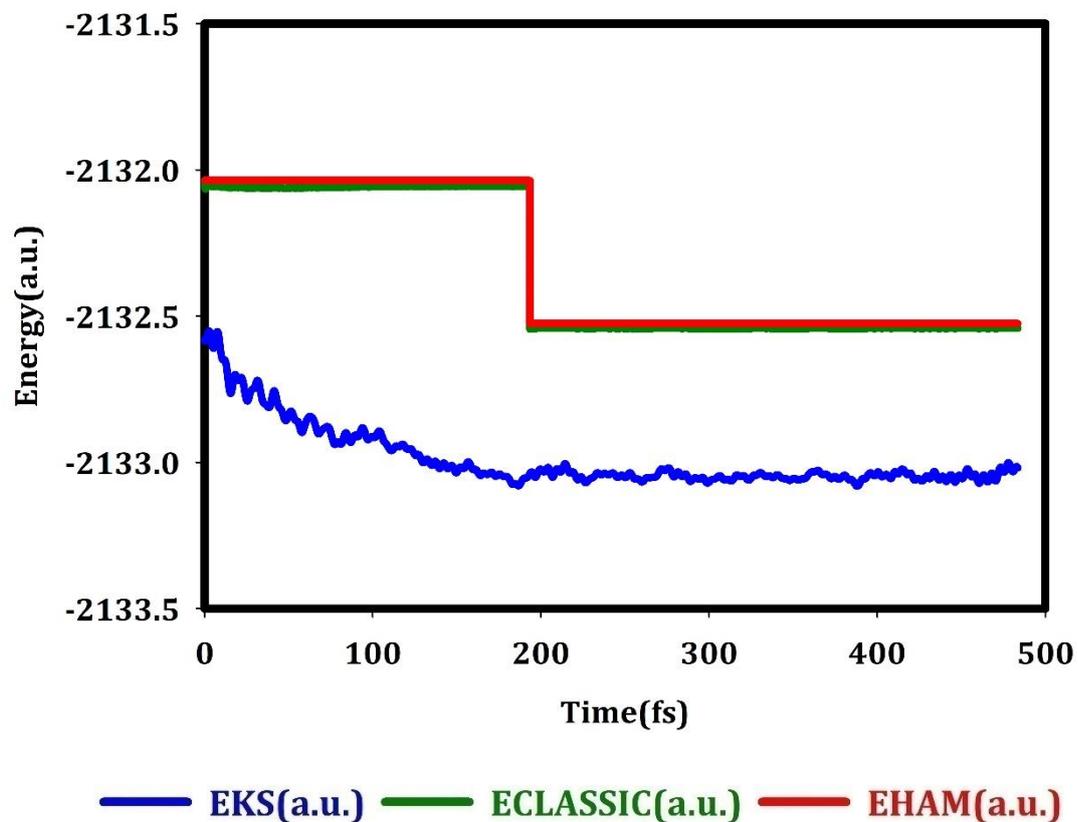
Supplementary Figure 6. The course of the fictitious kinetic energy of the electronic system and ionic temperature for Na^+ positioning in the center of graphene nanopore.
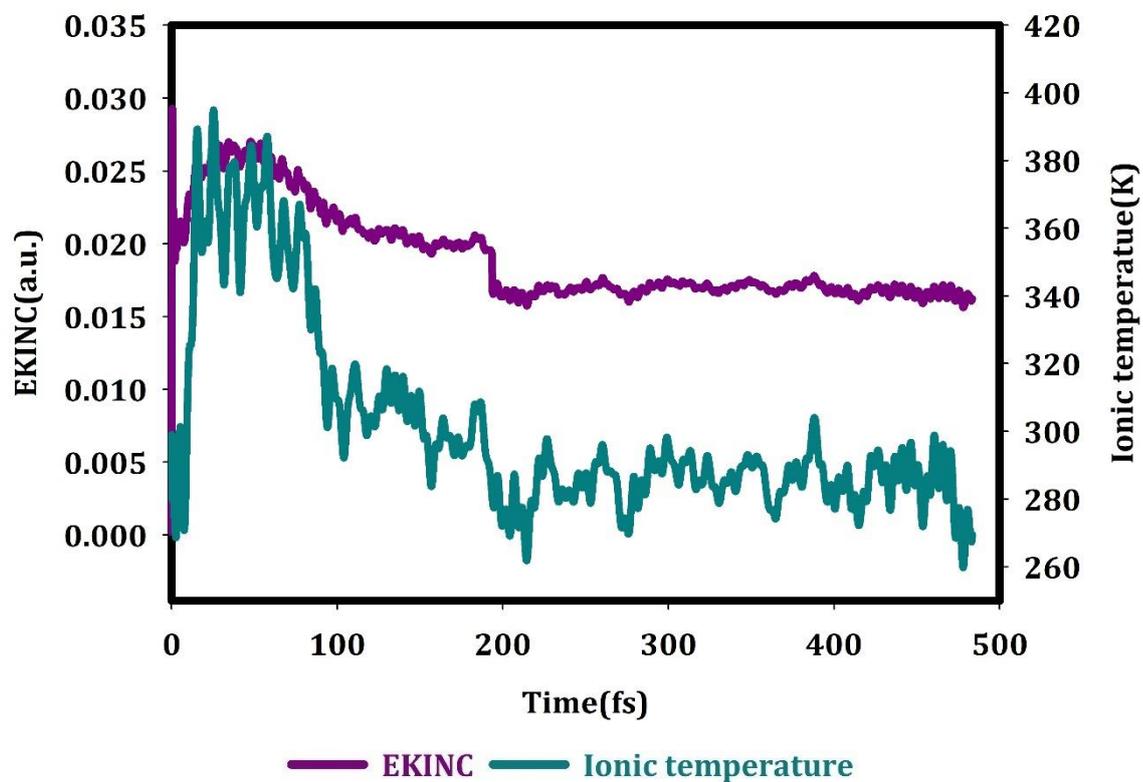
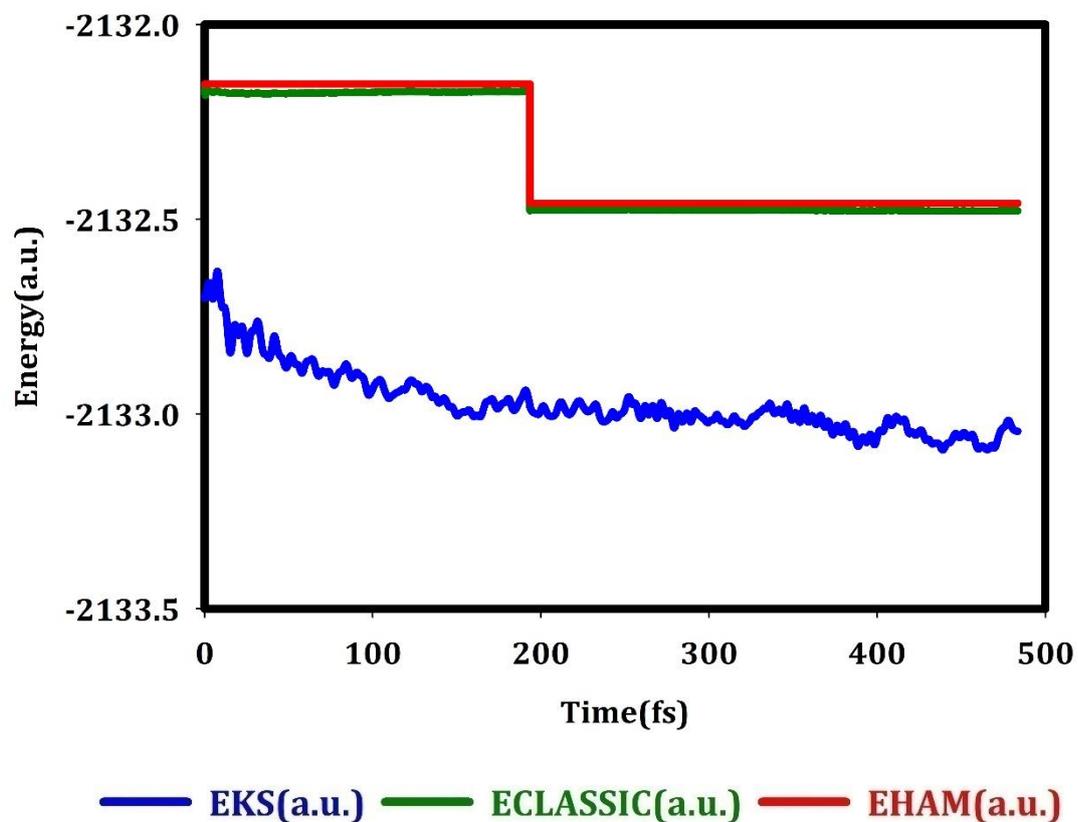Supplementary Figure 7. Energy courses for Na+ positioning at 3.5 Å above the center of graphene nanopore.

Supplementary Figure 8. The course of the fictitious kinetic energy of the electronic system and ionic temperature for Na+ positioning at 3.5 Å above the center of the graphene nanopore.
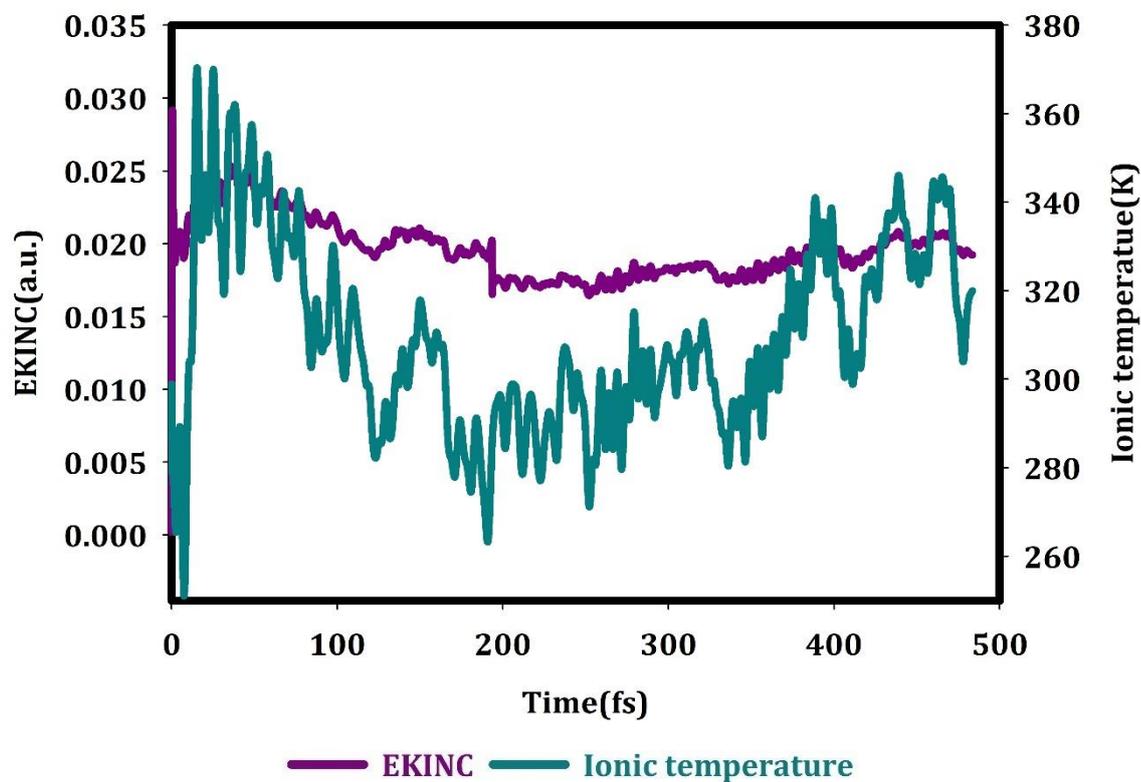
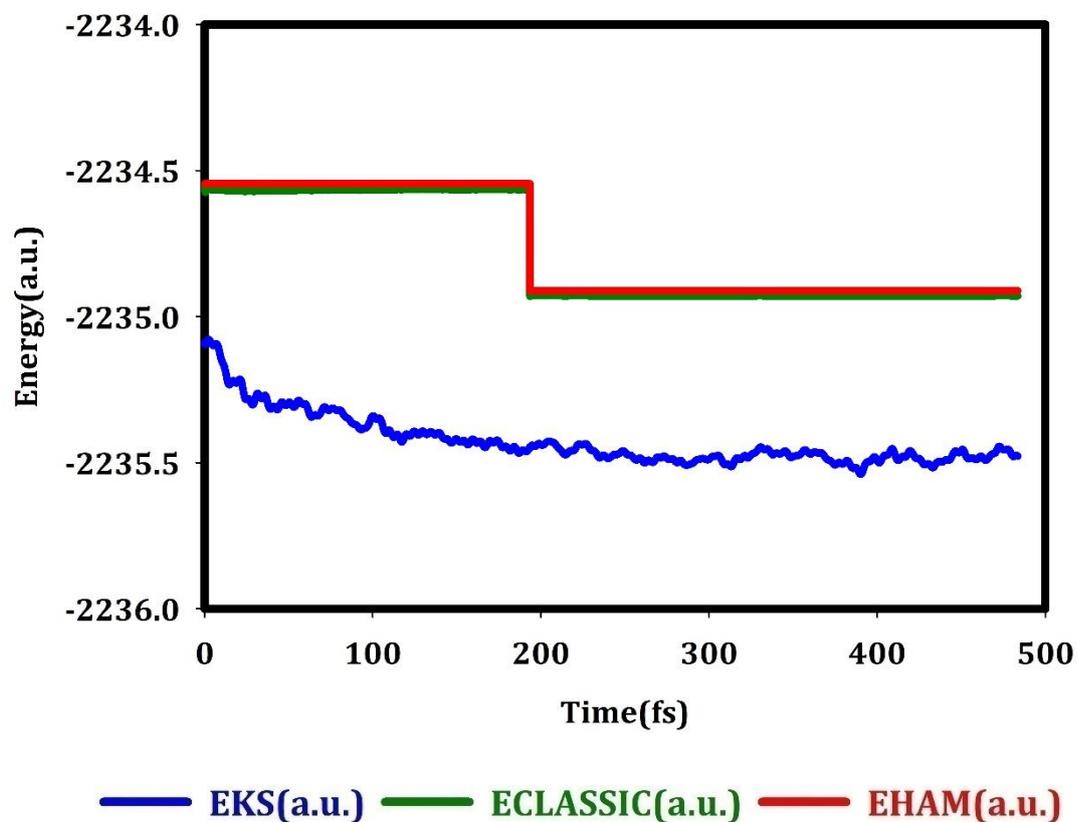Supplementary Figure 9.   Energy courses for Cl⁻ positioning in the center of the graphene nanopore.

Supplementary Figure 10. The course of the fictitious kinetic energy of the electronic system and ionic temperature for Cl^- positioning in the center of graphene nanopore.
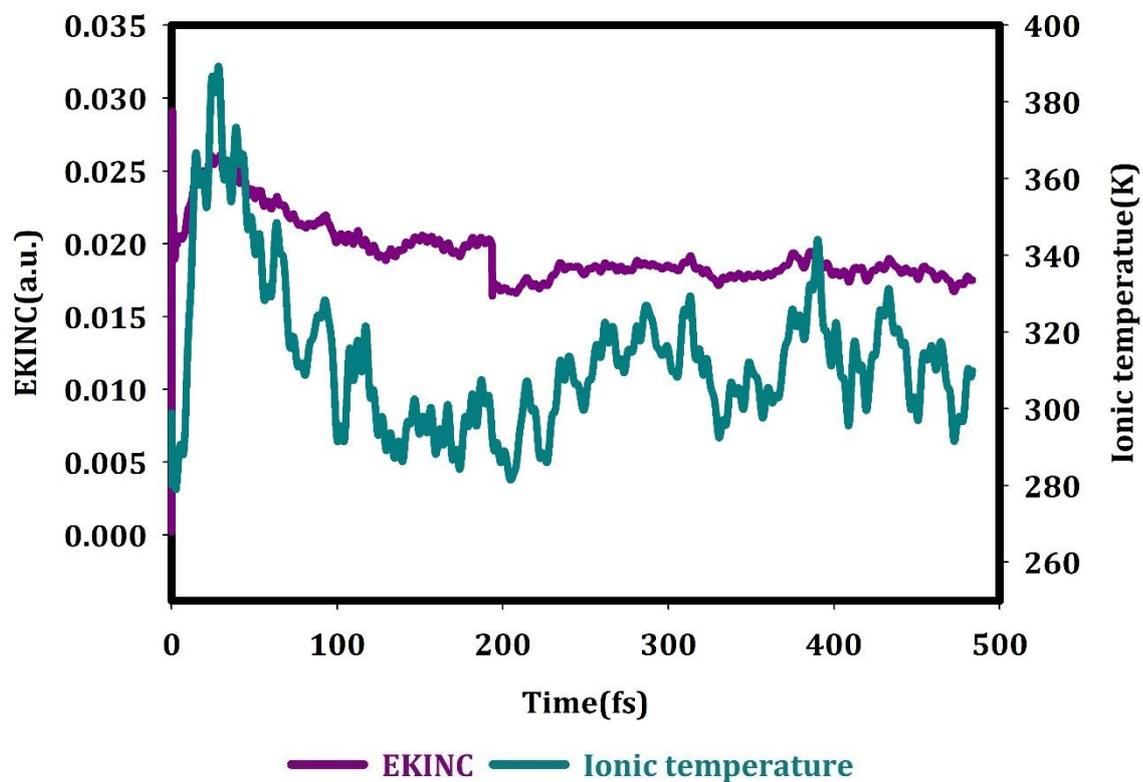
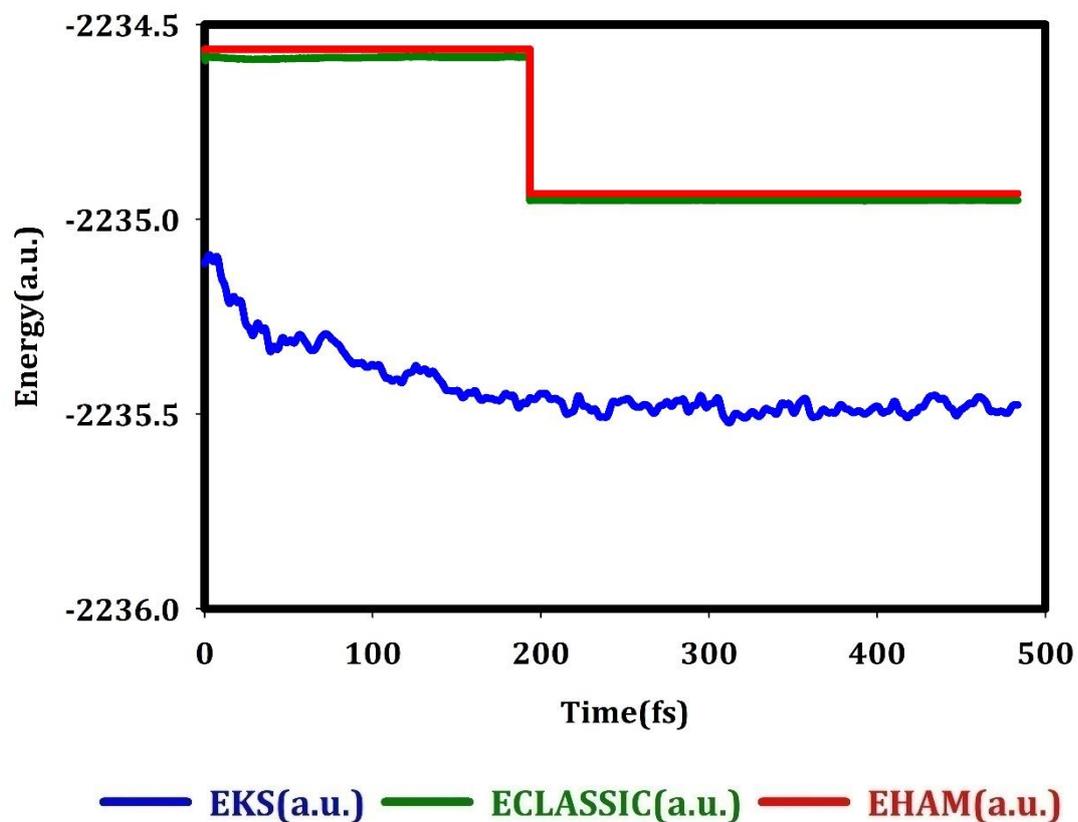Supplementary Figure 11. Energy courses for Cl⁻ positioning at 3.5 Å above the center of graphene nanopore.

Supplementary Figure 12. The course of the fictitious kinetic energy of the electronic system and ionic temperature for Cl⁻ positioning at 3.5 Å above the center of the graphene nanopore.
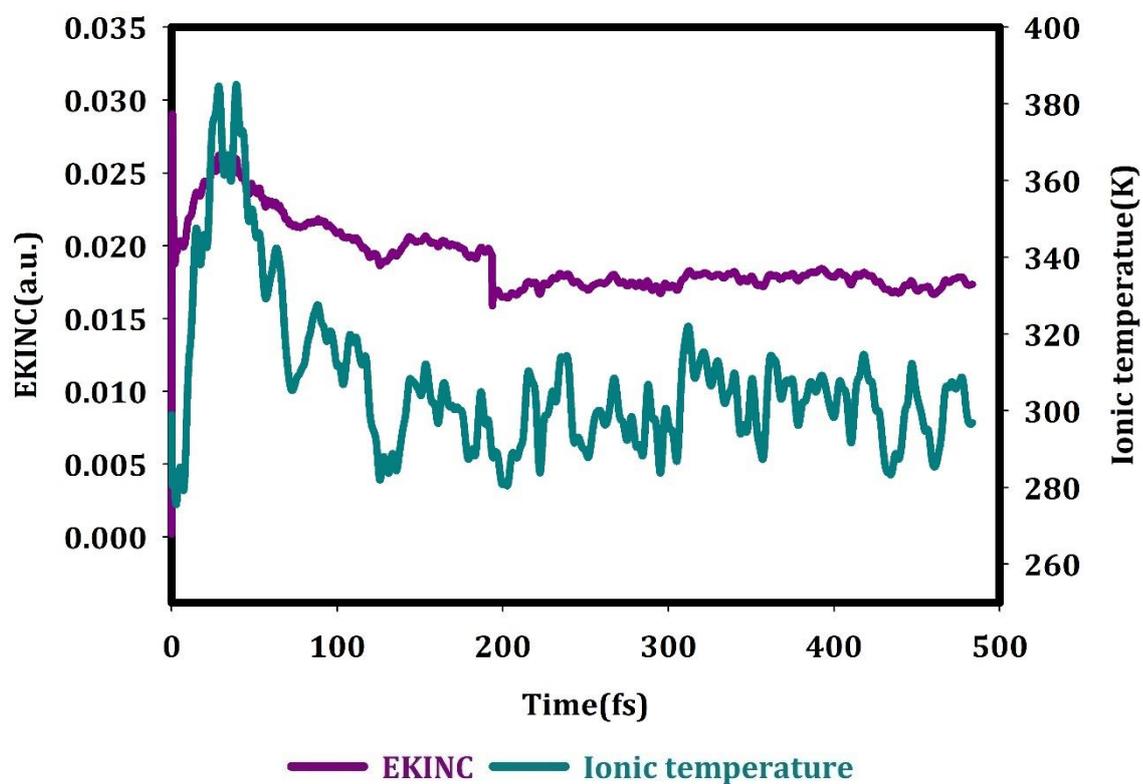
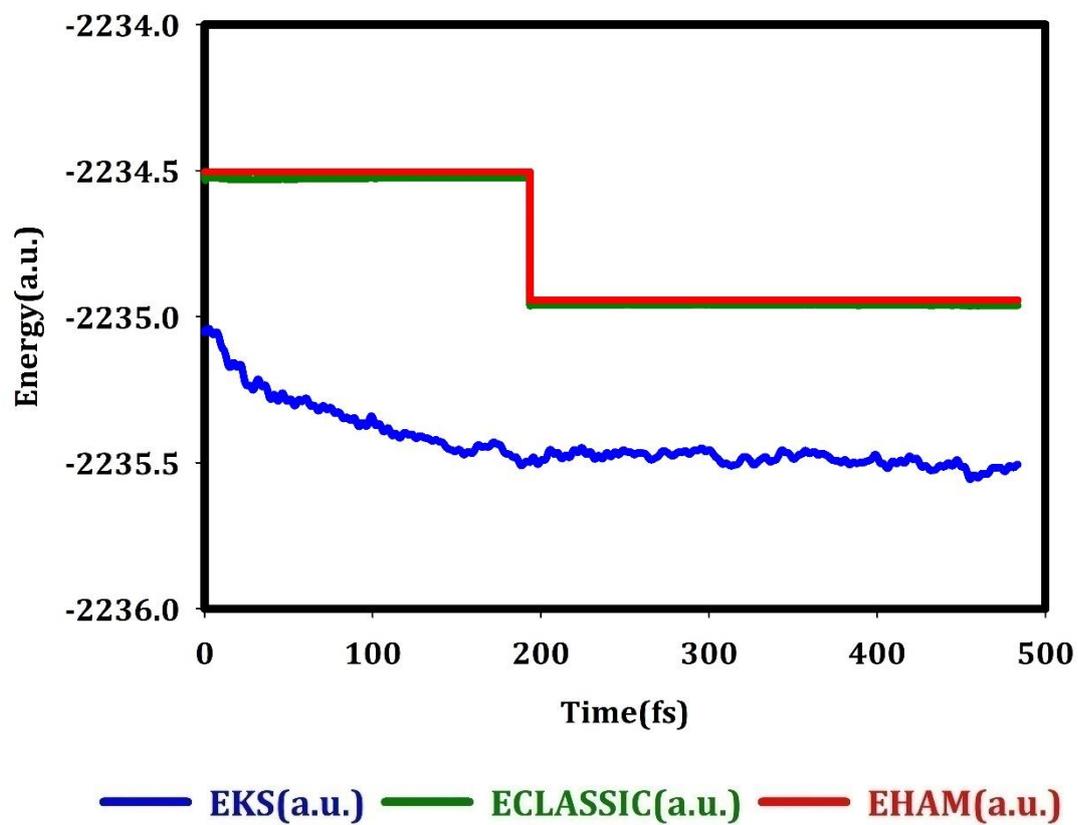Supplementary Figure 13. Energy courses for Na+ positioning in the center of the h-BN nanopore.

Supplementary Figure 14. The course of the fictitious kinetic energy of the electronic system and ionic temperature for Na+ positioning in the center of the h-BN nanopore.
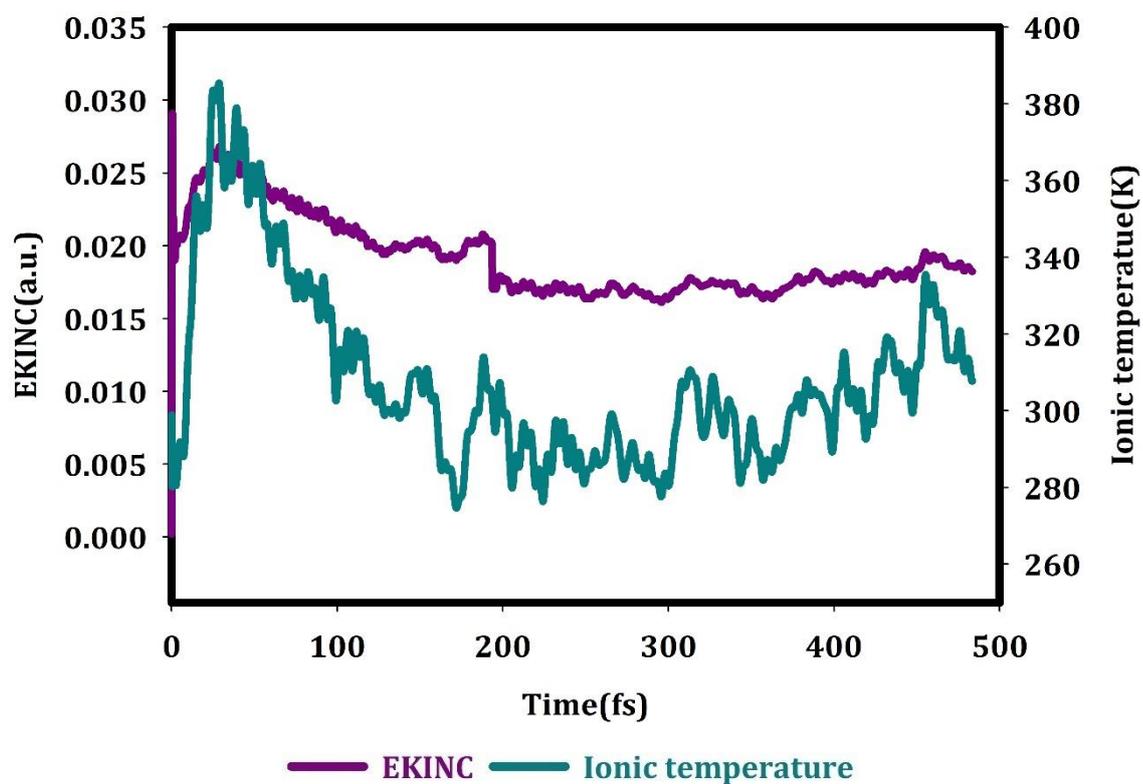
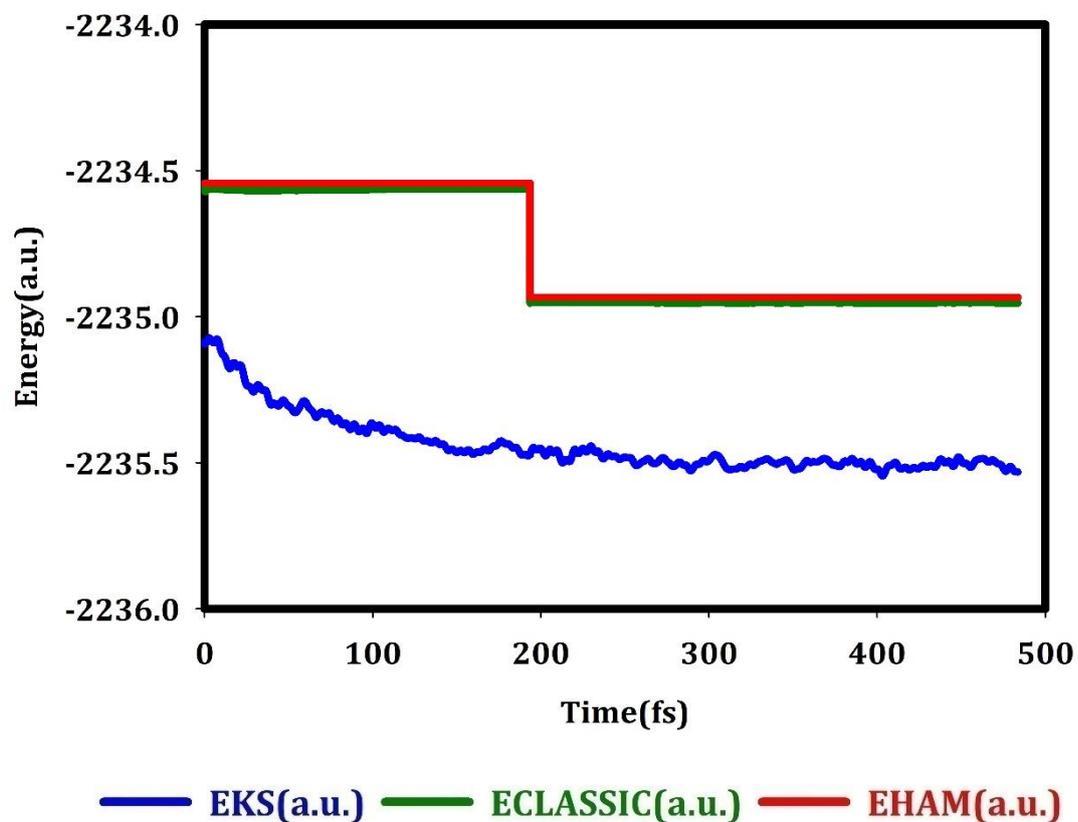Supplementary Figure 15. Energy courses for Na$^+$ positioning at 3.5 Å above the center of the h-BN nanopore.

Supplementary Figure 16. The course of the fictitious kinetic energy of the electronic system and ionic temperature for Na+ positioning at 3.5 Å above the center of the h-BN nanopore.
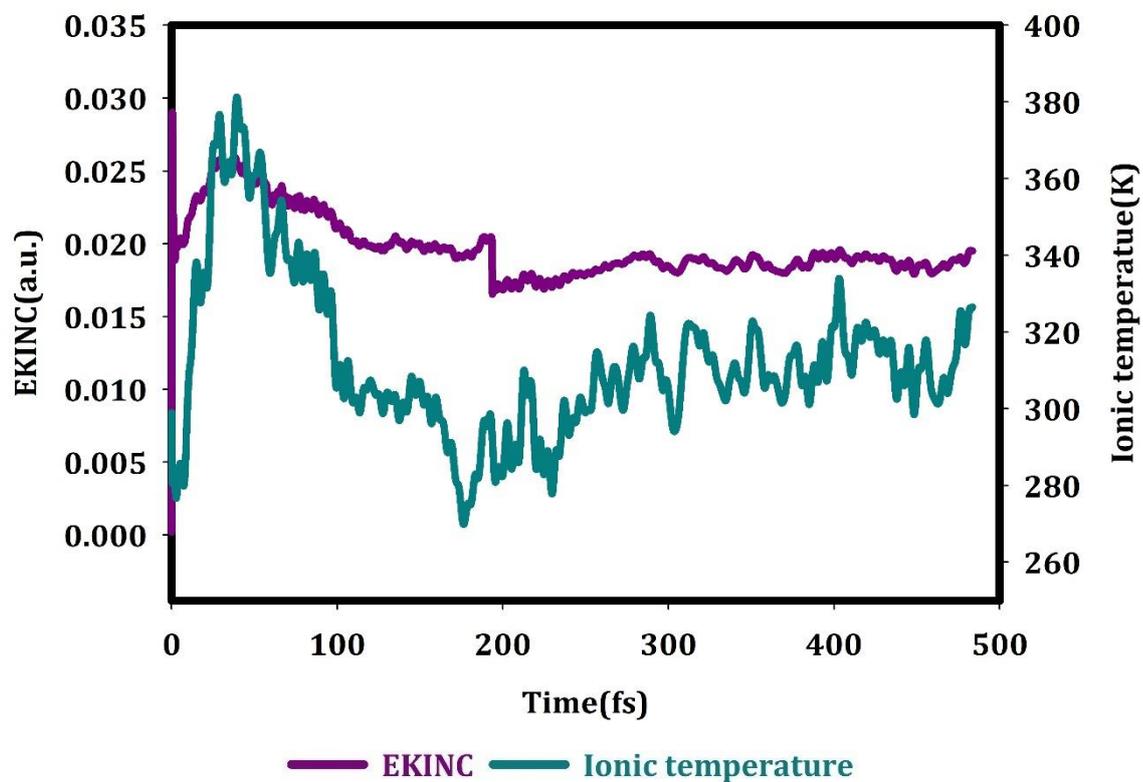
Supplementary Figure 17. Energy courses for Cl^- positioning in the center of the h-BN nanopore.

Supplementary Figure 18. The course of the fictitious kinetic energy of the electronic system and ionic temperature for Cl⁻ positioning in the center of the h-BN nanopore.

Supplementary Figure 19. Energy courses for Cl- positioning at 3.5 Å above the center of the h-BN nanopore.

Supplementary Figure 20. The course of the fictitious kinetic energy of the electronic system and ionic temperature for Cl- positioning at 3.5 Å above the center of the h-BN nanopore.