

Supporting Information for: Designing an All-Carbon Membrane for Water Desalination

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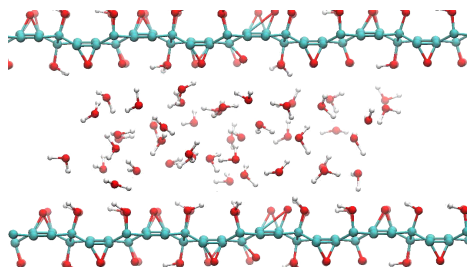
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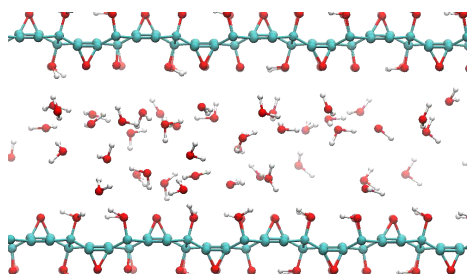
Material in the Supporting Information contains movies of molecular dynamics simulations that elucidate the permeation of water and Na^+ as well as K^+ ions in slit pores and through in-layer pores in graphene and GO. We compare in-layer pores representing the quasi-planar geometry of graphene and GO to pores with a staggered geometry that may occur at grain boundaries. All movies are linked directly to this pdf file.

A. Permeation of water molecules along slit pores in GO and graphene

Three layers of H_2O

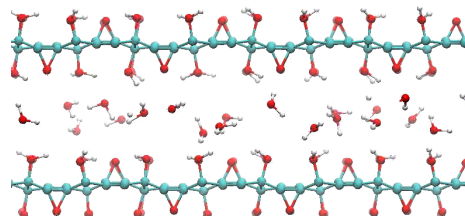


Video S1. Permeation of 3 layers of H_2O molecules along a slit pore in GO. All water molecules are subject to an external force characterized by $|\mathbf{F}_0| = 2.5 \times 10^{-2} \text{ eV/\AA}$.

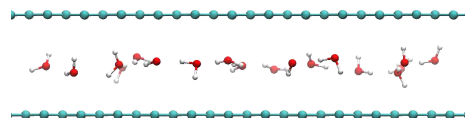


Video S2. Permeation of 3 layers of H_2O molecules along a slit pore in GO. All water molecules are subject to an external force characterized by $|\mathbf{F}_0| = 6.25 \times 10^{-3} \text{ eV/\AA}$.

One layer of H_2O



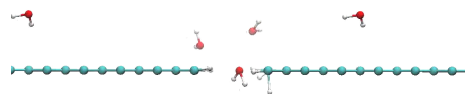
Video S3. Permeation of a monolayer of H_2O molecules along a slit pore in GO. All water molecules are subject to an external force characterized by $|\mathbf{F}_0| = 6.25 \times 10^{-3} \text{ eV/\AA}$.



Video S4. Permeation of a monolayer of H_2O molecules along a slit pore in graphite. All water molecules are subject to an external force characterized by $|\mathbf{F}_0| = 6.25 \times 10^{-3} \text{ eV/\AA}$.

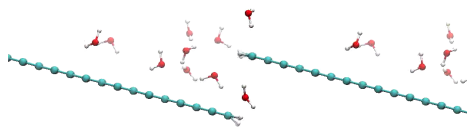
B. Permeation of water molecules through in-layer pores in graphene

H-terminated graphene armchair edges

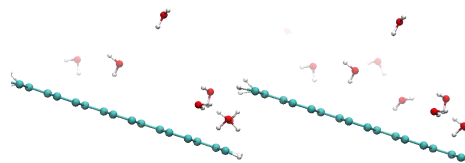


Video S5. Permeation of water molecules across a graphene in-layer pore with planar geometry and H-terminated armchair edges separated horizontally by $W = 5 \text{ \AA}$. All water molecules are subject to external forces characterized by $|\mathbf{F}_{0,\parallel}| = 6.25 \times 10^{-3} \text{ eV/\AA}$ acting along the layer and $|\mathbf{F}_{0,\perp}| = 6.25 \times 10^{-2} \text{ eV/\AA}$ acting normal to the layer.

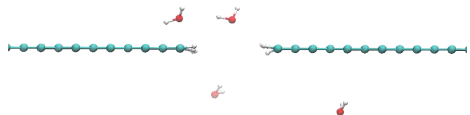
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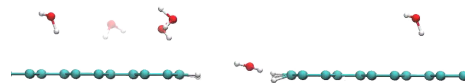
Video S6. Permeation of water molecules across a graphene in-layer pore with staggered geometry and H-terminated armchair edges separated vertically by $W = 5 \text{ \AA}$. All water molecules are subject to external forces characterized by $|\mathbf{F}_{\mathbf{o},\perp}| = 2.5 \times 10^{-2} \text{ eV/\AA}$ acting in vertical direction.



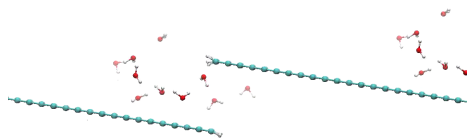
Video S10. Permeation of water molecules across a graphene in-layer pore with staggered geometry and H-terminated zigzag edges separated vertically by $W = 5 \text{ \AA}$. All water molecules are subject to external forces characterized by $|\mathbf{F}_{\mathbf{o},\perp}| = 2.5 \times 10^{-2} \text{ eV/\AA}$ acting in vertical direction.



Video S7. Permeation of water molecules across a graphene in-layer pore with planar geometry and H-terminated armchair edges separated horizontally by $W = 7 \text{ \AA}$. All water molecules are subject to external forces characterized by $|\mathbf{F}_{\mathbf{o},\parallel}| = 6.25 \times 10^{-3} \text{ eV/\AA}$ acting along the layer and $|\mathbf{F}_{\mathbf{o},\perp}| = 6.25 \times 10^{-2} \text{ eV/\AA}$ acting normal to the layer.

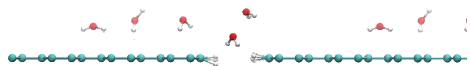


Video S11. Permeation of water molecules across a graphene in-layer pore with planar geometry and H-terminated zigzag edges separated horizontally by $W = 7 \text{ \AA}$. All water molecules are subject to external forces characterized by $|\mathbf{F}_{\mathbf{o},\parallel}| = 6.25 \times 10^{-3} \text{ eV/\AA}$ acting along the layer and $|\mathbf{F}_{\mathbf{o},\perp}| = 6.25 \times 10^{-2} \text{ eV/\AA}$ acting normal to the layer.

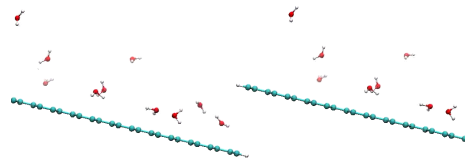


Video S8. Permeation of water molecules across a graphene in-layer pore with staggered geometry and H-terminated armchair edges separated vertically by $W = 7 \text{ \AA}$. All water molecules are subject to external forces characterized by $|\mathbf{F}_{\mathbf{o},\perp}| = 2.5 \times 10^{-2} \text{ eV/\AA}$ acting in vertical direction.

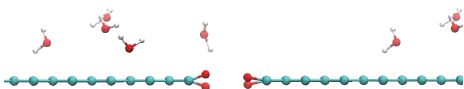
H-terminated graphene zigzag edges



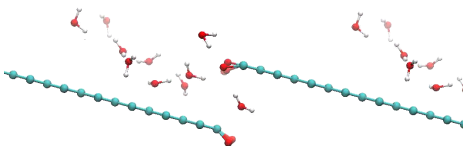
Video S9. Permeation of water molecules across a graphene in-layer pore with planar geometry and H-terminated zigzag edges separated horizontally by $W = 5 \text{ \AA}$. All water molecules are subject to external forces characterized by $|\mathbf{F}_{\mathbf{o},\parallel}| = 6.25 \times 10^{-3} \text{ eV/\AA}$ acting along the layer and $|\mathbf{F}_{\mathbf{o},\perp}| = 6.25 \times 10^{-2} \text{ eV/\AA}$



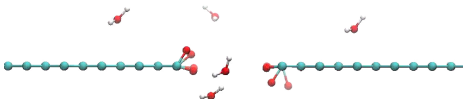
Video S12. Permeation of water molecules across a graphene in-layer pore with staggered geometry and H-terminated zigzag edges separated vertically by $W = 7 \text{ \AA}$. All water molecules are subject to external forces characterized by $|\mathbf{F}_{\mathbf{o},\perp}| = 2.5 \times 10^{-2} \text{ eV/\AA}$ acting in vertical direction.

O-terminated graphene armchair edges

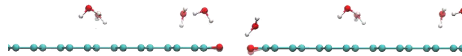
Video S13. Permeation of water molecules across a graphene in-layer pore with planar geometry and O-terminated armchair edges separated horizontally by $W = 5 \text{ \AA}$. All water molecules are subject to external forces characterized by $|\mathbf{F}_{\mathbf{o},\parallel}| = 6.25 \times 10^{-3} \text{ eV/\AA}$ acting along the layer and $|\mathbf{F}_{\mathbf{o},\perp}| = 6.25 \times 10^{-2} \text{ eV/\AA}$ acting normal to the layer.



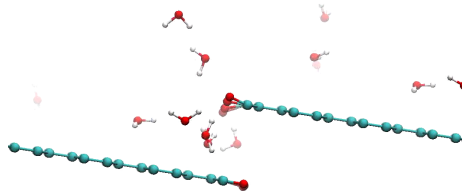
Video S14. Permeation of water molecules across a graphene in-layer pore with staggered geometry and O-terminated armchair edges separated vertically by $W = 5 \text{ \AA}$. All water molecules are subject to external forces characterized by $|\mathbf{F}_{\mathbf{o},\perp}| = 2.5 \times 10^{-2} \text{ eV/\AA}$ acting in vertical direction.



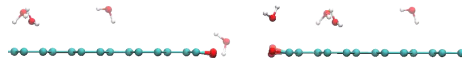
Video S15. Permeation of water molecules across a graphene in-layer pore with planar geometry and O-terminated armchair edges separated horizontally by $W = 7 \text{ \AA}$. All water molecules are subject to external forces characterized by $|\mathbf{F}_{\mathbf{o},\parallel}| = 6.25 \times 10^{-3} \text{ eV/\AA}$ acting along the layer and $|\mathbf{F}_{\mathbf{o},\perp}| = 6.25 \times 10^{-2} \text{ eV/\AA}$ acting normal to the layer.

O-terminated graphene zigzag edges

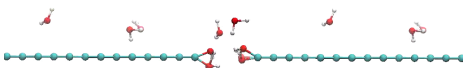
Video S16. Permeation of water molecules across a graphene in-layer pore with planar geometry and O-terminated zigzag edges separated horizontally by $W = 5 \text{ \AA}$. All water molecules are subject to external forces characterized by $|\mathbf{F}_{\mathbf{o},\parallel}| = 6.25 \times 10^{-3} \text{ eV/\AA}$ acting along the layer and $|\mathbf{F}_{\mathbf{o},\perp}| = 6.25 \times 10^{-2} \text{ eV/\AA}$ acting normal to the layer.



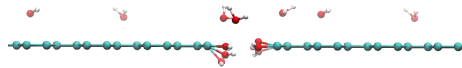
Video S17. Permeation of water molecules across a graphene in-layer pore with staggered geometry and O-terminated zigzag edges separated vertically by $W = 5 \text{ \AA}$. All water molecules are subject to external forces characterized by $|\mathbf{F}_{\mathbf{o},\perp}| = 2.5 \times 10^{-2} \text{ eV/\AA}$ acting in vertical direction.



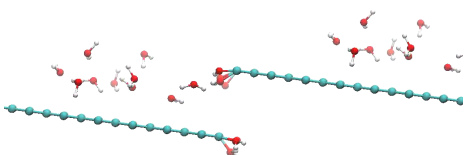
Video S18. Permeation of water molecules across a graphene in-layer pore with planar geometry and O-terminated zigzag edges separated horizontally by $W = 7 \text{ \AA}$. All water molecules are subject to external forces characterized by $|\mathbf{F}_{\mathbf{o},\parallel}| = 6.25 \times 10^{-3} \text{ eV/\AA}$ acting along the layer and $|\mathbf{F}_{\mathbf{o},\perp}| = 6.25 \times 10^{-2} \text{ eV/\AA}$ acting normal to the layer.

OH-terminated graphene armchair edges

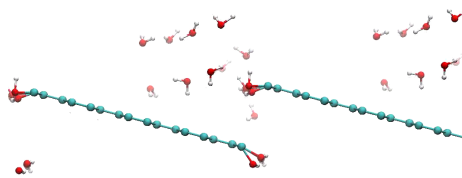
Video S19. Permeation of water molecules across a graphene in-layer pore with planar geometry and OH-terminated armchair edges separated horizontally by $W = 5 \text{ \AA}$. All water molecules are subject to external forces characterized by $|\mathbf{F}_{\mathbf{o},\parallel}| = 6.25 \times 10^{-3} \text{ eV/\AA}$ acting along the layer and $|\mathbf{F}_{\mathbf{o},\perp}| = 6.25 \times 10^{-2} \text{ eV/\AA}$ acting normal to the layer.

OH-terminated graphene zigzag edges

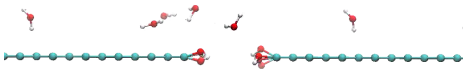
Video S22. Permeation of water molecules across a graphene in-layer pore with planar geometry and OH-terminated zigzag edges separated horizontally by $W = 5 \text{ \AA}$. All water molecules are subject to external forces characterized by $|\mathbf{F}_{\mathbf{o},\parallel}| = 6.25 \times 10^{-3} \text{ eV/\AA}$ acting along the layer and $|\mathbf{F}_{\mathbf{o},\perp}| = 6.25 \times 10^{-2} \text{ eV/\AA}$ acting normal to the layer.



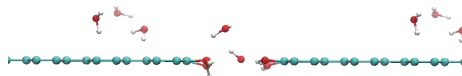
Video S20. Permeation of water molecules across a graphene in-layer pore with staggered geometry and OH-terminated armchair edges separated vertically by $W = 5 \text{ \AA}$. All water molecules are subject to external forces characterized by $|\mathbf{F}_{\mathbf{o},\perp}| = 2.5 \times 10^{-2} \text{ eV/\AA}$ acting in vertical direction.



Video S23. Permeation of water molecules across a graphene in-layer pore with staggered geometry and OH-terminated zigzag edges separated vertically by $W = 5 \text{ \AA}$. All water molecules are subject to external forces characterized by $|\mathbf{F}_{\mathbf{o},\perp}| = 2.5 \times 10^{-2} \text{ eV/\AA}$ acting in vertical direction.

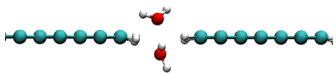


Video S21. Permeation of water molecules across a graphene in-layer pore with planar geometry and OH-terminated armchair edges separated horizontally by $W = 7 \text{ \AA}$. All water molecules are subject to external forces characterized by $|\mathbf{F}_{\mathbf{o},\parallel}| = 6.25 \times 10^{-3} \text{ eV/\AA}$ acting along the layer and $|\mathbf{F}_{\mathbf{o},\perp}| = 6.25 \times 10^{-2} \text{ eV/\AA}$ acting normal to the layer.

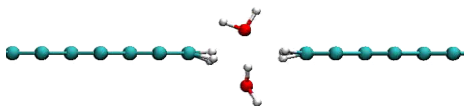


Video S24. Permeation of water molecules across a graphene in-layer pore with planar geometry and OH-terminated zigzag edges separated horizontally by $W = 7 \text{ \AA}$. All water molecules are subject to external forces characterized by $|\mathbf{F}_{\mathbf{o},\parallel}| = 6.25 \times 10^{-3} \text{ eV/\AA}$ acting along the layer and $|\mathbf{F}_{\mathbf{o},\perp}| = 6.25 \times 10^{-2} \text{ eV/\AA}$ acting normal to the layer.

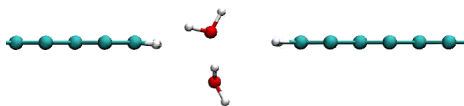
C. Concerted permeation of water molecules through in-layer pores in graphene



Video S25. Concerted permeation of water molecules across a graphene in-layer pore with planar geometry and H-terminated armchair edges separated horizontally by $W = 5 \text{ \AA}$. All water molecules are subject to external forces characterized by $|\mathbf{F}_{\mathbf{0},\perp}| = 2.5 \times 10^{-2} \text{ eV/\AA}$ acting normal to the layer.



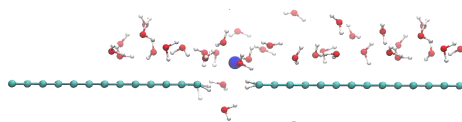
Video S26. Concerted permeation of water molecules across a graphene in-layer pore with planar geometry and H-terminated armchair edges separated horizontally by $W = 5 \text{ \AA}$. All water molecules are subject to external forces characterized by $|\mathbf{F}_{\mathbf{0},\perp}| = 6.25 \times 10^{-3} \text{ eV/\AA}$ acting normal to the layer.



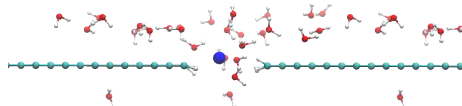
Video S27. Concerted permeation of water molecules across a graphene in-layer pore with planar geometry and H-terminated armchair edges separated horizontally by $W = 7 \text{ \AA}$. All water molecules are subject to external forces characterized by $|\mathbf{F}_{\mathbf{0},\perp}| = 6.25 \times 10^{-3} \text{ eV/\AA}$ acting normal to the layer.

D. Permeation of hydrated Na^+ ions through in-layer pores in graphene and GO

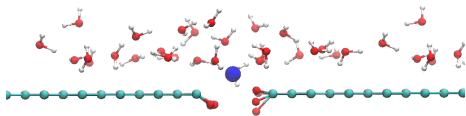
H-terminated graphene armchair edges



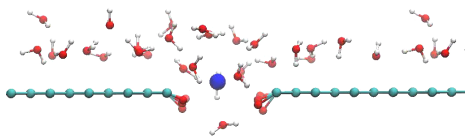
Video S28. Permeation of hydrated Na^+ ions across a graphene in-layer pore with planar geometry and H-terminated armchair edges separated horizontally by $W = 5 \text{ \AA}$. All water molecules and Na^+ ion are subject to external forces characterized by $|\mathbf{F}_{\mathbf{0},\parallel}| = 6.25 \times 10^{-3} \text{ eV/\AA}$ acting along the layer and $|\mathbf{F}_{\mathbf{0},\perp}| = 2.5 \times 10^{-2} \text{ eV/\AA}$ acting normal to the layer.



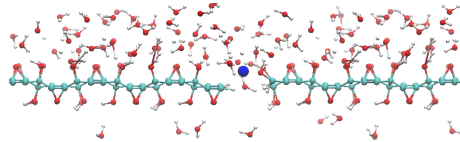
Video S29. Permeation of hydrated Na^+ ions across a graphene in-layer pore with planar geometry and H-terminated armchair edges separated horizontally by $W = 7 \text{ \AA}$. All water molecules and Na^+ ion are subject to external forces characterized by $|\mathbf{F}_{\mathbf{0},\parallel}| = 6.25 \times 10^{-3} \text{ eV/\AA}$ acting along the layer and $|\mathbf{F}_{\mathbf{0},\perp}| = 2.5 \times 10^{-2} \text{ eV/\AA}$ acting normal to the layer.

O-terminated graphene armchair edges

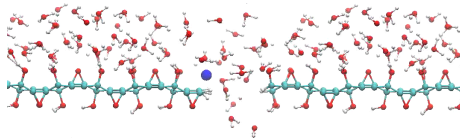
Video S30. Permeation of hydrated Na^+ ions across a graphene in-layer pore with planar geometry and O-terminated armchair edges separated horizontally by $W = 5 \text{ \AA}$. All water molecules and Na^+ ion are subject to external forces characterized by $|\mathbf{F}_{\mathbf{o},\parallel}| = 6.25 \times 10^{-3} \text{ eV/\AA}$ acting along the layer and $|\mathbf{F}_{\mathbf{o},\perp}| = 2.5 \times 10^{-2} \text{ eV/\AA}$ acting normal to the layer.



Video S31. Permeation of hydrated Na^+ ions across a graphene in-layer pore with planar geometry and O-terminated armchair edges separated horizontally by $W = 7 \text{ \AA}$. All water molecules and Na^+ ion are subject to external forces characterized by $|\mathbf{F}_{\mathbf{o},\parallel}| = 6.25 \times 10^{-3} \text{ eV/\AA}$ acting along the layer and $|\mathbf{F}_{\mathbf{o},\perp}| = 2.5 \times 10^{-2} \text{ eV/\AA}$ acting normal to the layer.

H-terminated GO armchair edges

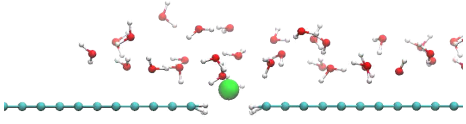
Video S32. Permeation of hydrated Na^+ ions across a GO in-layer pore with planar geometry and H-terminated armchair edges separated horizontally by $W = 5 \text{ \AA}$. All water molecules and Na^+ ion are subject to external forces characterized by $|\mathbf{F}_{\mathbf{o},\parallel}| = 6.25 \times 10^{-3} \text{ eV/\AA}$ acting along the layer and $|\mathbf{F}_{\mathbf{o},\perp}| = 2.5 \times 10^{-2} \text{ eV/\AA}$ acting normal to the layer.



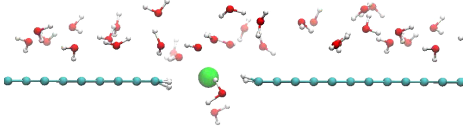
Video S33. Permeation of hydrated Na^+ ions across a GO in-layer pore with planar geometry and H-terminated armchair edges separated horizontally by $W = 7 \text{ \AA}$. All water molecules and Na^+ ion are subject to external forces characterized by $|\mathbf{F}_{\mathbf{o},\parallel}| = 6.25 \times 10^{-3} \text{ eV/\AA}$ acting along the layer and $|\mathbf{F}_{\mathbf{o},\perp}| = 2.5 \times 10^{-2} \text{ eV/\AA}$ acting normal to the layer.

E. Permeation of hydrated K^+ ions through in-layer pores in graphene

H-terminated graphene armchair edges

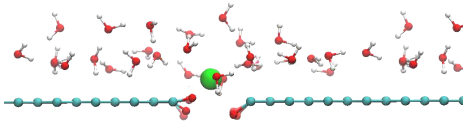


Video S34. Permeation of hydrated K^+ ions across a graphene in-layer pore with planar geometry and H-terminated armchair edges separated horizontally by $W = 5 \text{ \AA}$. All water molecules and K^+ ion are subject to external forces characterized by $|\mathbf{F}_{0,\parallel}| = 6.25 \times 10^{-3} \text{ eV/\AA}$ acting along the layer and $|\mathbf{F}_{0,\perp}| = 2.5 \times 10^{-2} \text{ eV/\AA}$ acting normal to the layer.

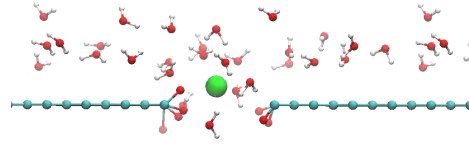


Video S35. Permeation of hydrated K^+ ions across a graphene in-layer pore with planar geometry and H-terminated armchair edges separated horizontally by $W = 7 \text{ \AA}$. All water molecules and K^+ ion are subject to external forces characterized by $|\mathbf{F}_{0,\parallel}| = 6.25 \times 10^{-3} \text{ eV/\AA}$ acting along the layer and $|\mathbf{F}_{0,\perp}| = 2.5 \times 10^{-2} \text{ eV/\AA}$ acting normal to the layer.

O-terminated graphene armchair edges



Video S36. Permeation of hydrated K^+ ions across a graphene in-layer pore with planar geometry and O-terminated armchair edges separated horizontally by $W = 5 \text{ \AA}$. All water molecules and K^+ ion are subject to external forces characterized by $|\mathbf{F}_{0,\parallel}| = 6.25 \times 10^{-3} \text{ eV/\AA}$ acting along the layer and $|\mathbf{F}_{0,\perp}| = 2.5 \times 10^{-2} \text{ eV/\AA}$ acting normal to the layer.



Video S37. Permeation of hydrated K^+ ions across a graphene in-layer pore with planar geometry and O-terminated armchair edges separated horizontally by $W = 7 \text{ \AA}$. All water molecules and K^+ ion are subject to external forces characterized by $|\mathbf{F}_{0,\parallel}| = 6.25 \times 10^{-3} \text{ eV/\AA}$ acting along the layer and $|\mathbf{F}_{0,\perp}| = 2.5 \times 10^{-2} \text{ eV/\AA}$ acting normal to the layer.