Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

First principles studies of the interactions between alkali metal elements and oxygen-passivated nanopores in graphene (Supplemental Information)

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Charge Distribution

Here we provide plots of the charge transfer for Li (Fig. 1-3), Na (Fig. 4-6), and K (Fig. 7-9) adsorption onto pristine graphene and the five nanopores considered in the study. The charge transfer δq at each atom is given by $\delta q = q_{P+AM} - q_P - q_{AM}$ where q_{P+AM}, q_P, and q_{AM} represent the local atomic charges within the combined alkali-nanopore sheet, lone porous sheet, and lone alkali metal, respectively. The atomic charges are estimated using the Löwdin population analysis under the projected DOS method. Plots labeled (a) and (b) in Fig. 1-9 are top-down perspectives of the local charges in two graphene membranes while plots labeled (c) and (d) are the radial charge distributions away from the adsorbates.

Case for Li:

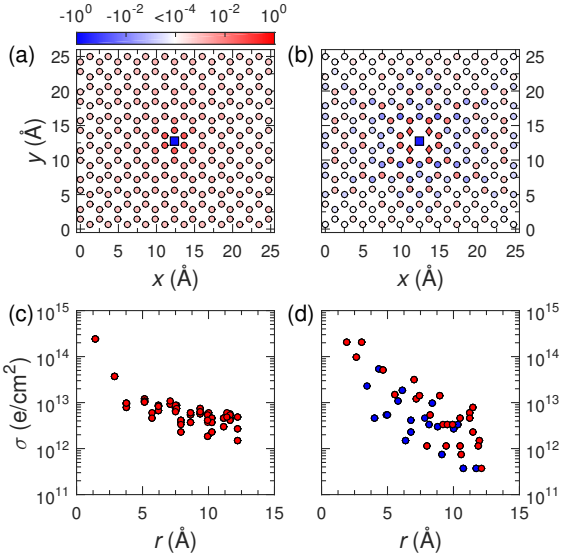

Figure 1: Charge distribution on (a,c) pristine graphene and (b,d) nanopore 6-4O after Li adsorption.

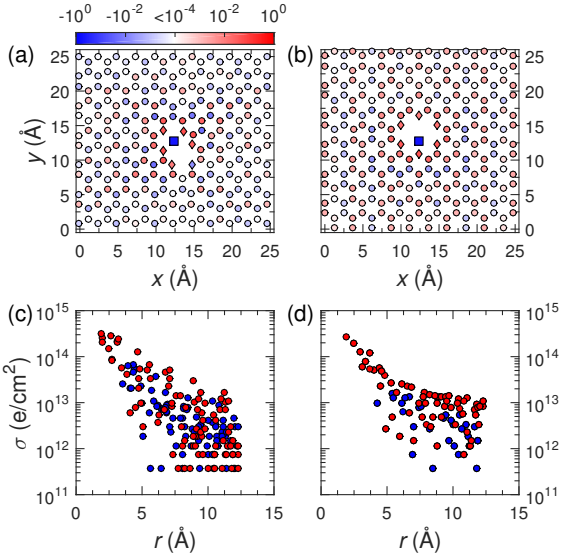

Figure 2: Charge distribution on (a,c) nanopore 10-6O and (b,d) nanopore 12-6O after Li adsorption.

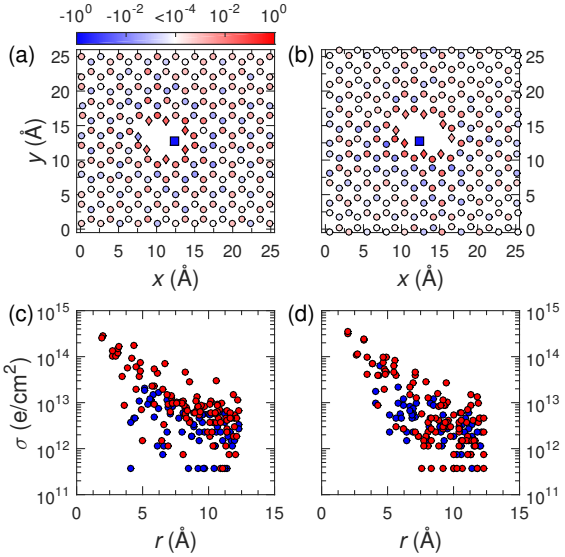

Figure 3: Charge distribution on (a,c) nanopore 14-7O and (b,d) nanopore 16-8O after Li adsorption.

Case for Na:

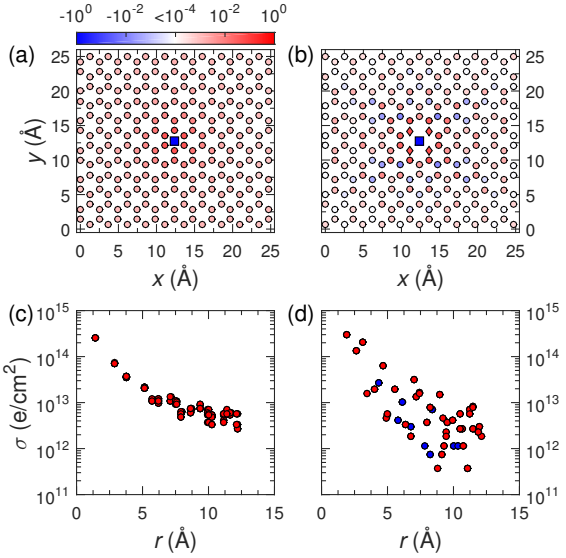

Figure 4: Charge distribution on (a,c) pristine graphene and (b,d) nanopore 6-4O after Na adsorption.

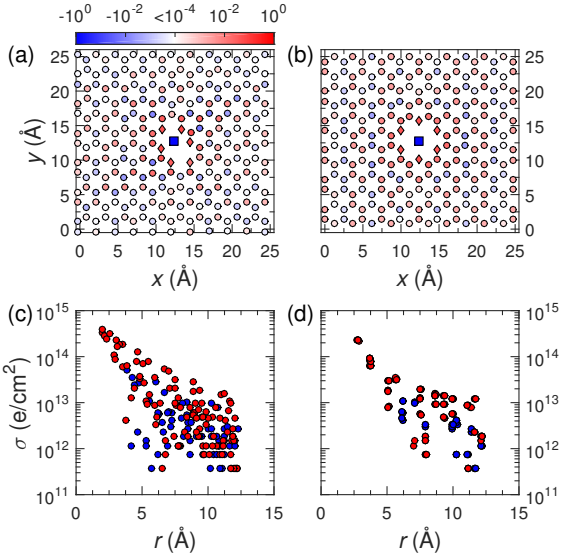

Figure 5: Charge distribution on (a,c) nanopore 10-6O and (b,d) nanopore 12-6O after Na adsorption.

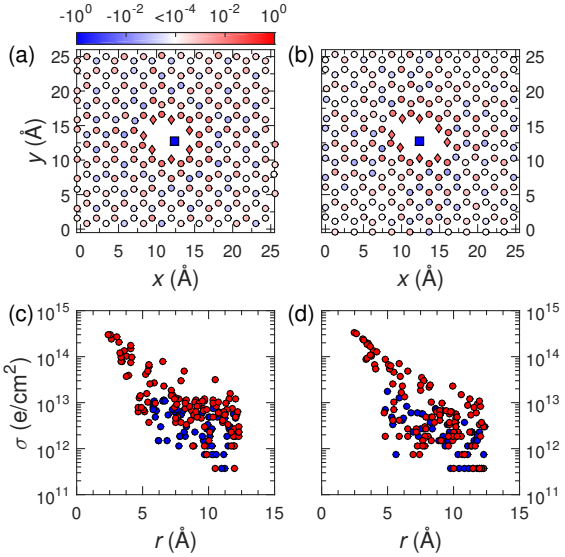

Figure 6: Charge distribution on (a,c) nanopore 14-7O and (b,d) nanopore 16-8O after Na adsorption.

Case for K:

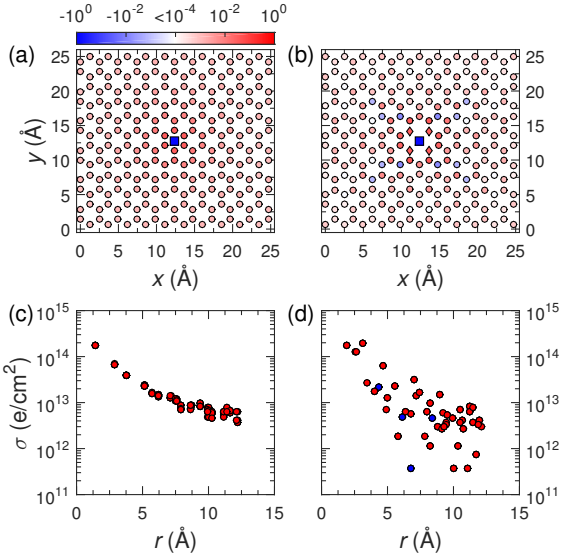

Figure 7: Charge distribution on (a,c) pristine graphene and (b,d) nanopore 6-4O after K adsorption.

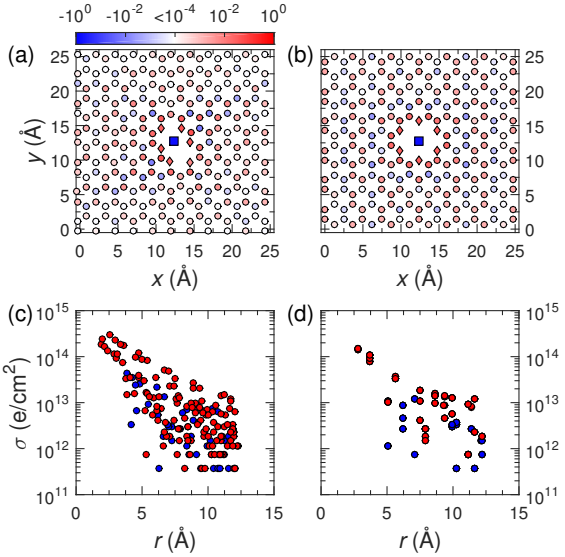

Figure 8: Charge distribution on (a,c) nanopore 10-6O and (b,d) nanopore 12-6O after K adsorption.

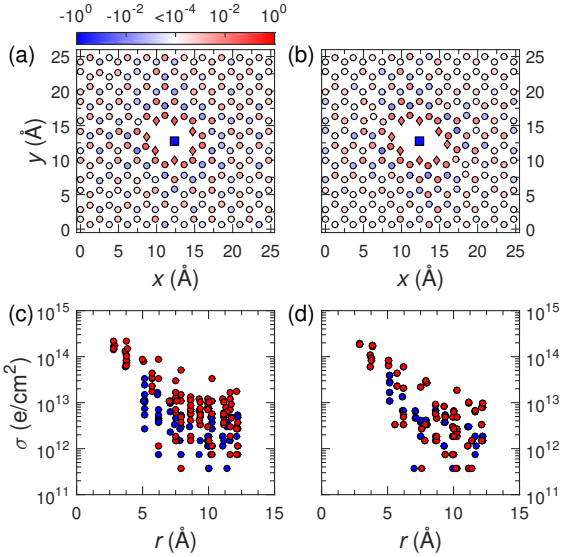

Figure 9: Charge distribution on (a,c) nanopore 14-7O and (b,d) nanopore 16-8O after K adsorption.

Electronic Structure

Here we provide the electronic band structures for pristine graphene [Fig. 10(a)] and a membrane with nanopore 12-6O [Fig. 10(b)] before (black bands) and after (red bands) Na adsorption. A small band gap is seen in the electronic structure of the graphene sheet containing the functionalized nanopore [Fig. 10(b)]. Moreover, we observe a rigid band shift in pristine and functionalized graphene states after Na adsorption as shown in Fig. 10

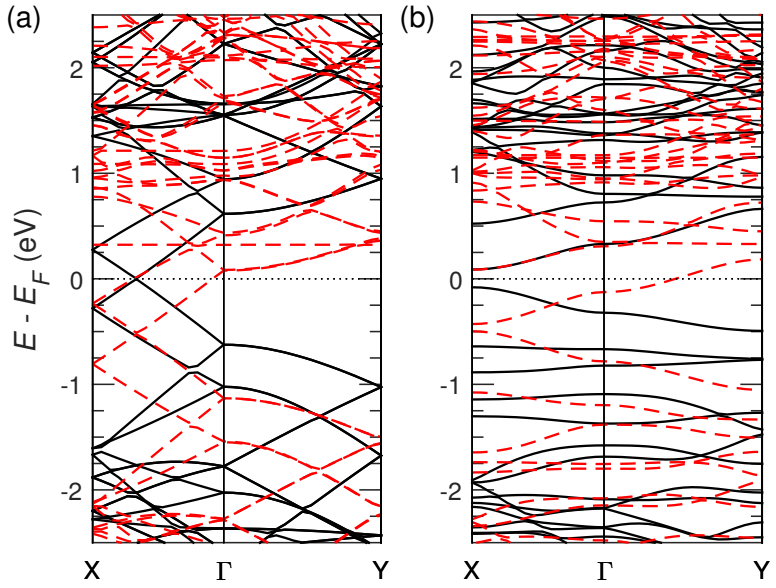

Figure 10: (a) Electronic band structure of pristine garphene before (black) and after (red) Na adsorption. (b) Electronic band structure of nanopore 12-6O before (black) and after (red) Na adsorption. The graphene sheet containing nanopore 12-6O produces a small band gap.

Work Function

Here we provide the work functions [Fig. 11(a)] and Fermi energies [Fig. 11(b)] of pristine graphene and the five nanopores considered in this study before and after alkali metal adsorption. We include dashed lines within the plots [Fig. 11(a) and Fig. 11(b)] to help guide the eye.

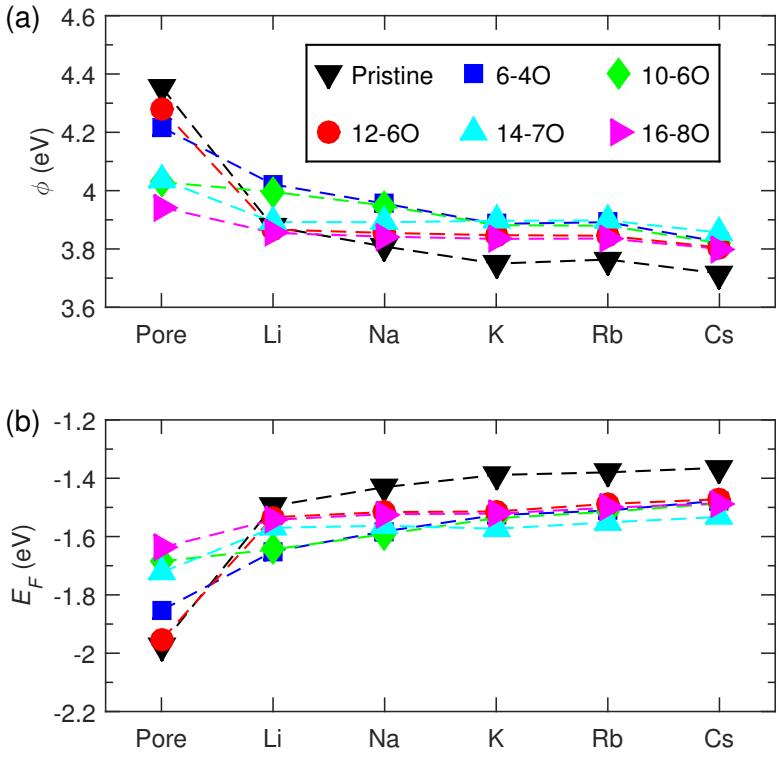

Figure 11: (a) Pristine graphene exhibits a larger work function compared to functionalized membranes. After alkali adsorption, the work function decreases for all porous sheets. (b) The Fermi energy for graphene and functionalized membranes changes alongside the work function.