Understanding doping strategies in the design of organic electrode materials for Li and Na ion batteries: an electronic structure perspective

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The computed formation energies for the lithiation and sodiation of the coronene, the deprotonated phenalene, the phenalene, the disodium terephthalate and the disodium naphthalate molecules are shown in Figure 1 and 2 (lithiation) and Figure 3 and 4 (sodiation), respectively. The formation energies were computed according to Eq. (1) in the main article. In Figure 1 to 4, the strongest interactions between Li/Na atoms and the molecules are shown by blue circles. The other computed formation energies are shown as black crosses in Figure 1 to 4.

Figure 5 to Figure 9 show the structures of lithium attached onto coronene, deprotonated phenalene, phenalene, disodium terephthalate and disodium naphthalate, respectively, with the lowest energy. Figure 10 to Figure 14 show the structures of the sodiated coronene, deprotonated phenalene, phenalene, disodium terephthalate and disodium naphthalate, respectively, with the lowest energy. The subfigures in each row show the attachment of an increasing number of Li/Na atoms from left to right. For each structure, a top and a side view is given. Hydrogen atoms are shown in white, lithium atoms in orange, boron atoms in pink, carbon atoms in grey, nitrogen atoms in blue and sodium atoms in green. The formation energies of these structures correspond to the blue circles in Figure 1 to 4.
Figure 1: Formation energies of all computed lithiated structures. The energies are shown for a) coronene, b) phenalene, c) deprotonated phenalene and their doped versions indicated by their chemical formula. The minimal formation energies are marked by filled blue circles and all other energies by black crosses.
a) Disodium terephthalate + Li

b) Disodium naphthalate + Li

Figure 2: Formation energies of all computed lithiated structures. The energies are shown for a) disodium terephthalate, e) disodium naphthalate and their doped versions indicated by their chemical formula. The minimal formation energies are marked by filled blue circles and all other energies by black crosses.
Figure 3: Formation energies of all computed sodiated structures. The energies are shown for a) coronene, b) phenalene, c) deprotonated phenalene and their doped versions indicated by their chemical formula. The minimal formation energies are marked by filled blue circles and all other energies by black crosses.
Figure 4: Formation energies of all computed sodiated structures. The energies are shown for a) disodium terephthalate, e) disodium naphthalate and their doped versions indicated by their chemical formula. The minimal formation energies are marked by filled blue circles and all other energies by black crosses.
Figure 5: Lowest energy structures of the lithiated coronene molecule and its doped versions. The attachment of $n$ Li atoms on a) triple p-doped, b) p-doped, c) pristine, d) n-doped and e) triple n-doped coronene is shown. The number of Li atoms ($n$) increases from left to right. For each structure, a top and a side view is given.
Figure 6: Lowest energy structures of the lithiated deprotonated phenalene molecule and its doped versions. The attachment of n Li atoms on a) triple p-doped, b) p-doped, c) pristine, d) n-doped and e) triple n-doped deprotonated phenalene molecule is shown. The number of Li atoms (n) increases from left to right. For each structure, a top and a side view is given.
Figure 7: Lowest energy structures of the lithiated phenalene molecule and its doped versions. The attachment of $n$ Li atoms on a) triple p-doped, b) p-doped, c) pristine, d) n-doped and e) triple n-doped phenalene molecule is shown. The number of Li atoms ($n$) increases from left to right. For each structure, a top and a side view is given.
Figure 8: Lowest energy structures of the lithiated disodium terephthalate and its doped versions. The attachment of n Li atoms on a) p-doped version 2 (v2), b) pristine and c) n-doped version 2 (v2) disodium terephthalate is shown. The number of Li atoms increases from left to right. For each structure, a top and a side view is given.
Figure 9: Lowest energy structures of the lithiated disodium naphthalate and its doped versions. The attachment of n Li atoms on a) p-doped version 1 (v1), b) p-doped version 2 (v2), c) p-doped version 3 (v3), d) pristine, e) n-doped version 1 (v1), f) n-doped version 2 (v2) and g) n-doped version 3 (v3) disodium naphthalate is shown. The number of Li atoms (n) increases from left to right. For each structure, a top and a side view is given.
Figure 10: Lowest energy structures of the sodiated coronene molecule and its doped versions. The attachment of $n$ Na atoms on a) triple p-doped, b) p-doped, c) pristine, d) n-doped and e) triple n-doped coronene is shown. The number of Na atoms ($n$) increases from left to right. For each structure, a top and a side view is given.
Figure 11: Lowest energy structures of the sodiated deprotonated phenalene molecule and its doped versions. The attachment of n Na atoms on a) triple p-doped, b) p-doped, c) pristine, d) n-doped and e) triple n-doped deprotonated phenalene molecule is shown. The number of Na atoms (n) increases from left to right. For each structure, a top and a side view is given.
Figure 12: Lowest energy structures of the sodiated phenalene molecule and its doped versions. The attachment of $n$ Na atoms on a) triple p-doped, b) p-doped, c) pristine, d) n-doped and e) triple n-doped phenalene molecule is shown. The number of Na atoms ($n$) increases from left to right. For each structure, a top and a side view is given.
Figure 13: Lowest energy structures of the sodiated disodium terephthalate and its doped versions. The attachment of $n$ Na atoms on a) p-doped version 2 (v2), b) pristine and c) n-doped version 2 (v2) disodium terephthalate is shown. The number of Na atoms increases from left to right. For each structure, a top and a side view is given.
Figure 14: Lowest energy structures of the sodiated disodium naphthalate and its doped versions. The attachment of n Na atoms on a) p-doped version 1 (v1), b) p-doped version 2 (v2), c) p-doped version 3 (v3), d) pristine, e) n-doped version 1 (v1), f) n-doped version 2 (v2) and g) n-doped version 3 (v3) disodium naphthalate is shown. The number of Na atoms (n) increases from left to right. For each structure, a top and a side view is given.