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# *Selective Separation Behavior of Graphene Flake in Interaction with Halide Anions in the Presence of External Electric Field*

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## Supporting Information

| Table S1. The HOMO, LUMO, and HOMO-LUMO band gap energies corresponding to the investigated molecular systems at the M06-2X/6-31G (d,p) level of theory. | | | | |
|---|---|---|---|---|
| **Molecular Complexes** | **Electric Field Strength (au)** | **HOMO Orbital Energies (eV)** | **LUMO Orbital Energies (eV)** | **HOMO-LUMO Band Gap (eV)** |
| $C_{54}H_{18}$ | 0.0000 | -5.95 | -1.6 | 4.35 |
| | 0.0005 | -5.95 | -1.6 | 4.35 |
| | 0.0010 | -5.95 | -1.6 | 4.35 |
| | 0.0015 | -5.95 | -1.6 | 4.35 |
| | 0.0020 | -5.95 | -1.6 | 4.35 |
| | 0.0030 | -5.95 | -1.6 | 4.35 |
| $C_{54}H_{18}F^-$ | 0.0000 | -2.42 | 1.02 | 3.44 |
| | 0.0005 | -2.45 | 1.01 | 3.46 |
| | 0.0010 | -2.46 | 1.01 | 3.47 |
| | 0.0015 | -2.47 | 1.01 | 3.48 |
| | 0.0020 | -2.47 | 1.01 | 3.48 |
| | 0.0030 | -2.49 | 1.00 | 3.49 |
| $C_{54}H_{18}Cl^-$ | 0.0000 | -2.13 | 0.73 | 2.86 |
| | 0.0005 | -2.14 | 0.69 | 2.83 |
| | 0.0010 | -2.19 | 0.70 | 2.89 |
| | 0.0015 | -2.23 | 0.69 | 2.92 |
| | 0.0020 | -2.92 | 0.23 | 3.15 |
| | 0.0030 | -2.93 | 0.23 | 3.16 |
| $C_{54}H_{18}Br^-$ | 0.0000 | -1.81 | 0.73 | 2.54 |
| | 0.0005 | -1.86 | 0.70 | 2.56 |
| | 0.0010 | -1.91 | 0.70 | 2.61 |
| | 0.0015 | -1.95 | 0.69 | 2.64 |
| | 0.0020 | -1.98 | 0.65 | 2.63 |
| | 0.0030 | -2.09 | 0.65 | 2.74 |