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Solid State Zwitterions realized on carbon graphenic surface ZHAOHUI HUANG, VINCENT CRESPI, Dept.of Physics,Penn State Univ. — Zwitterions are single molecular species that combine anionic and cationic groups. Here we consider the prospects for introducing the concept of a zwitterion into the solid state, by combining geometrically incompatible anionic and cationic moieties within a single extended structural element whose covalent rigidity frustrates the close approach of the anionic and cationic regions. Specifically, first principles computations for anionic and cationic groups such as NH3 and CO2 covalently attached to a graphenic surface via linker elements demonstrate long-range charge transfer, the hallmark of a zwitterion, while maintaining overall structural integrity.

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