

Ab initio study of MoS₂-graphene heterostructure for metal atoms intercalation

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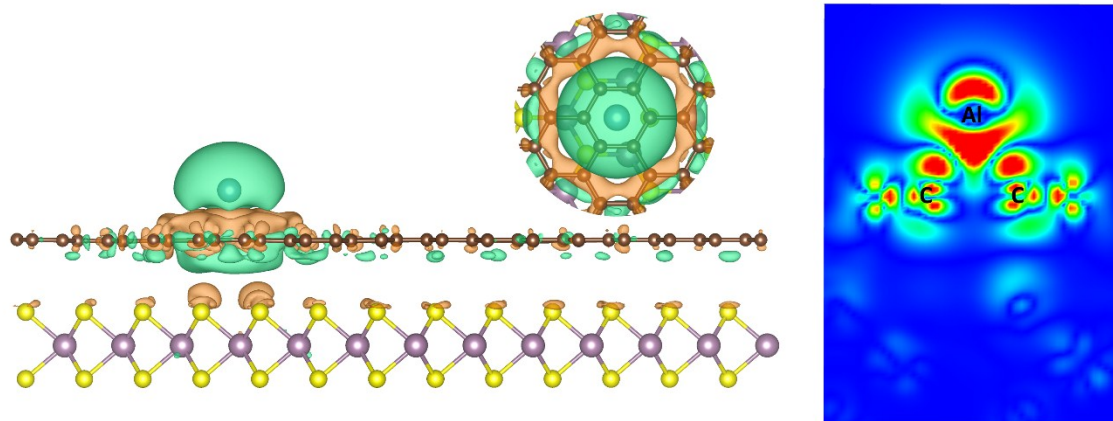
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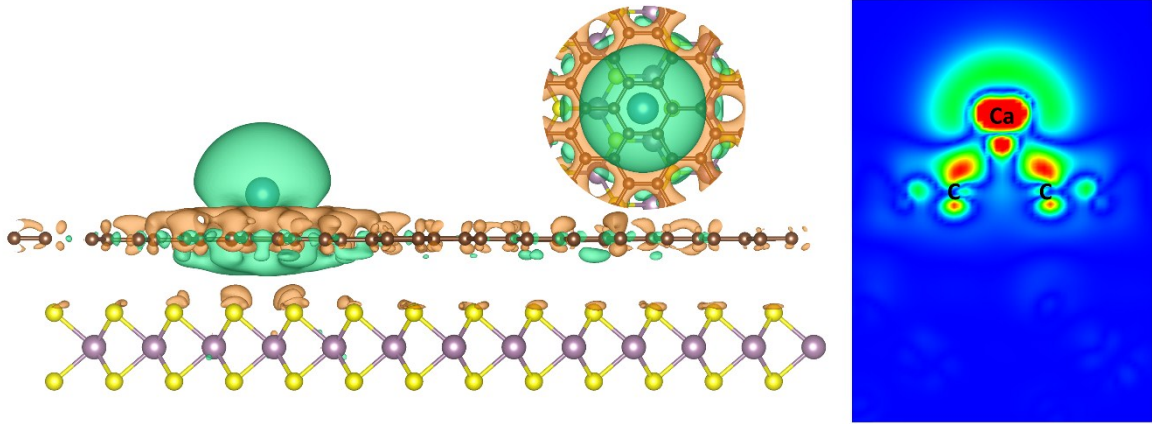
Supporting Information

G_{side}:

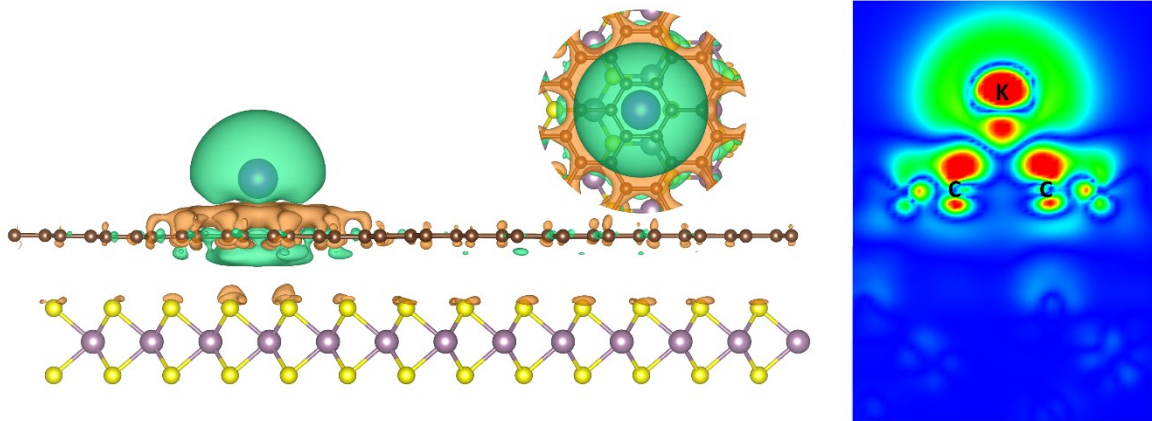
Al



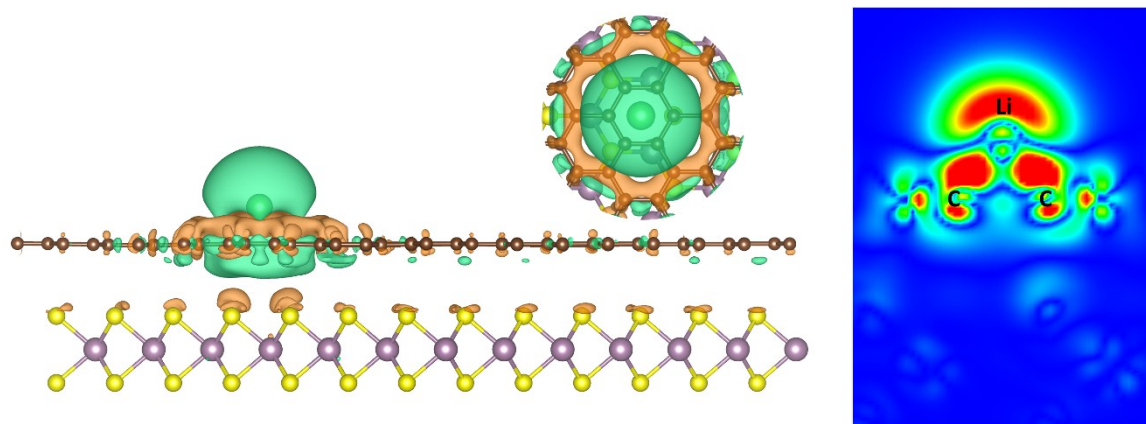
Ca



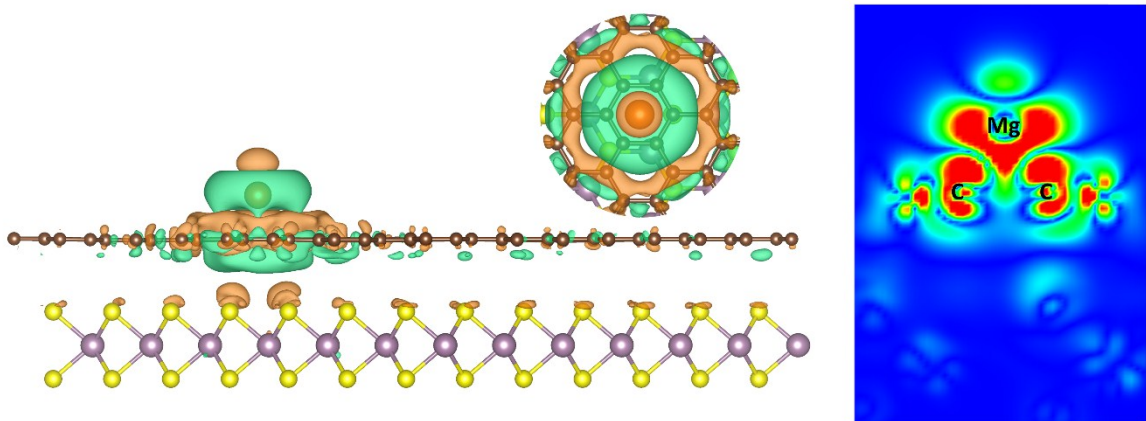
K



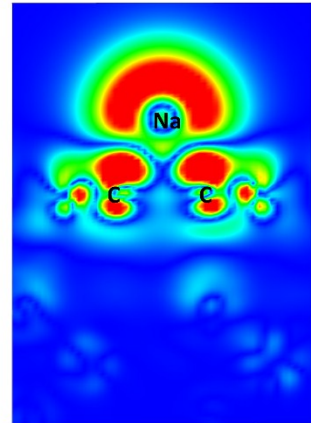
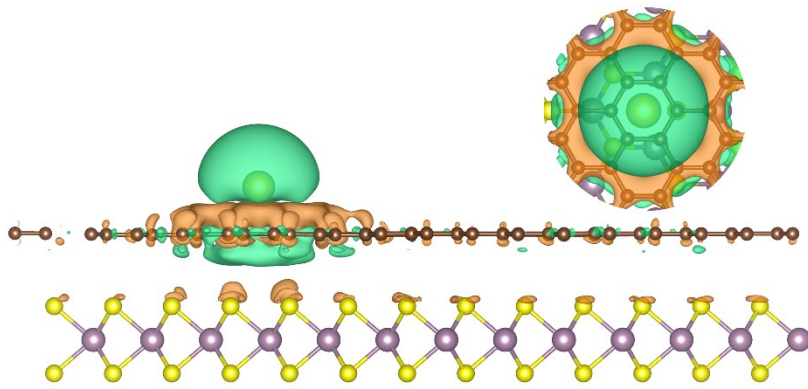
Li



Mg

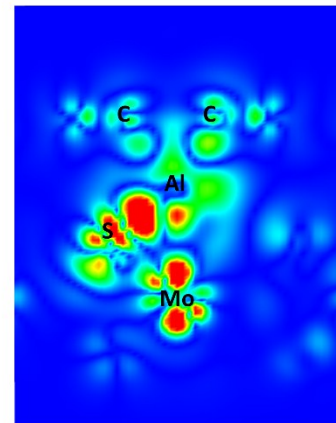
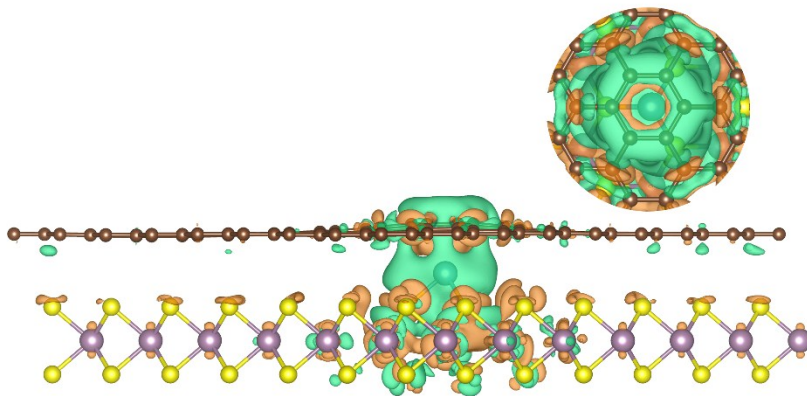


Na

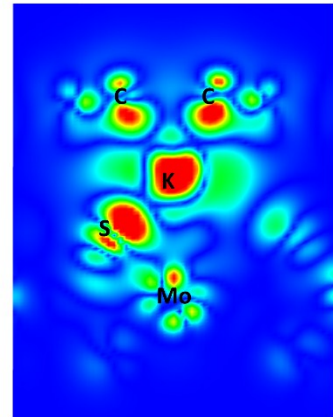
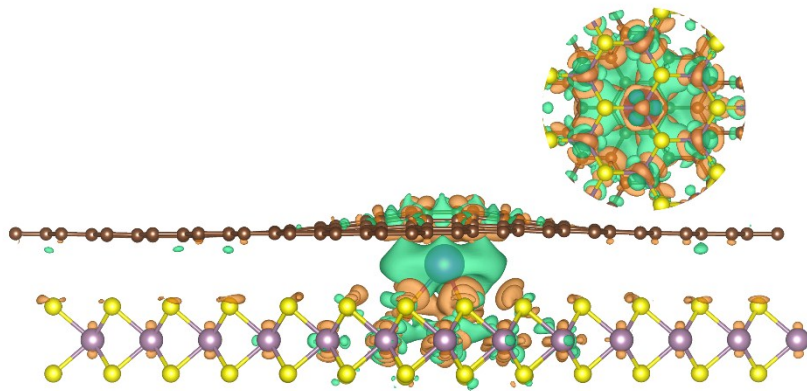


Interlayer:

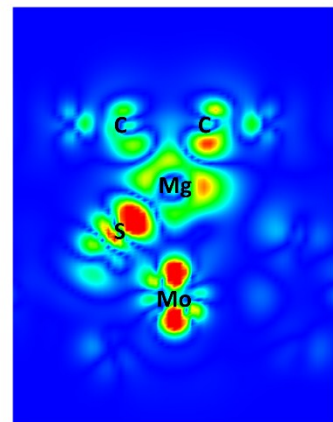
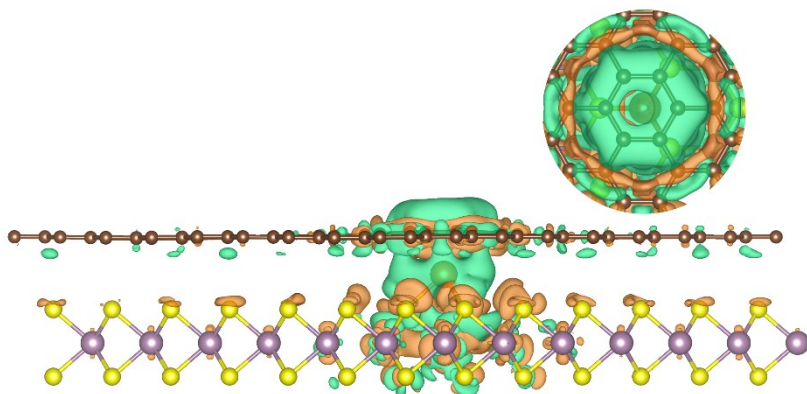
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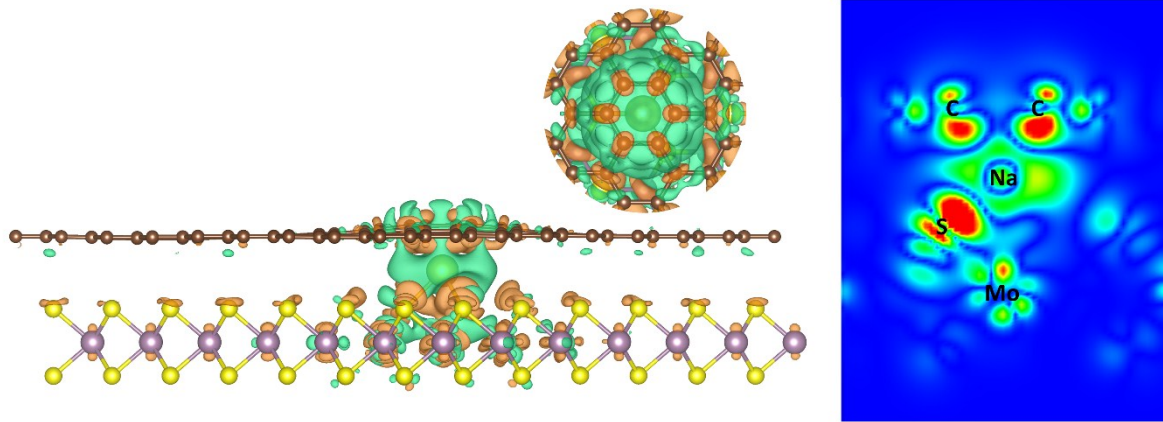
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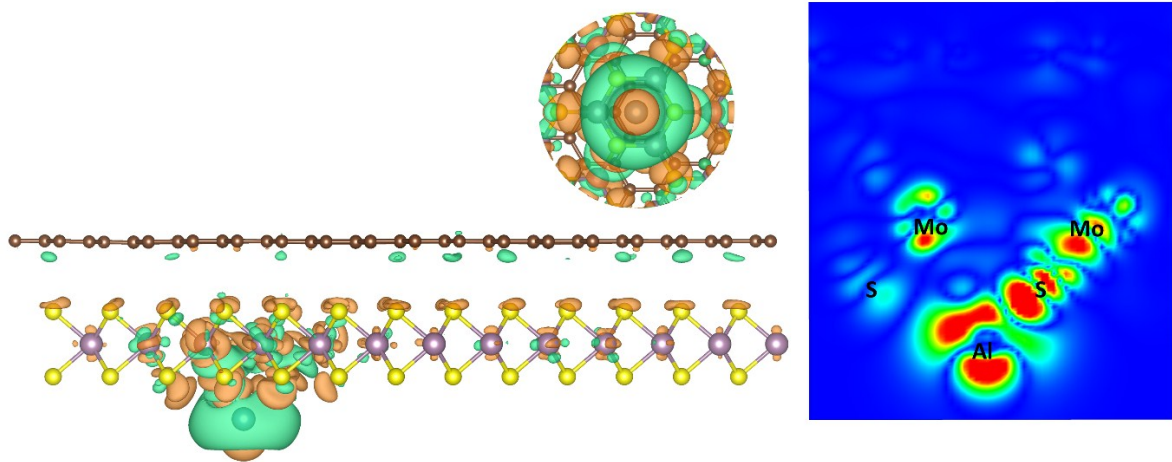


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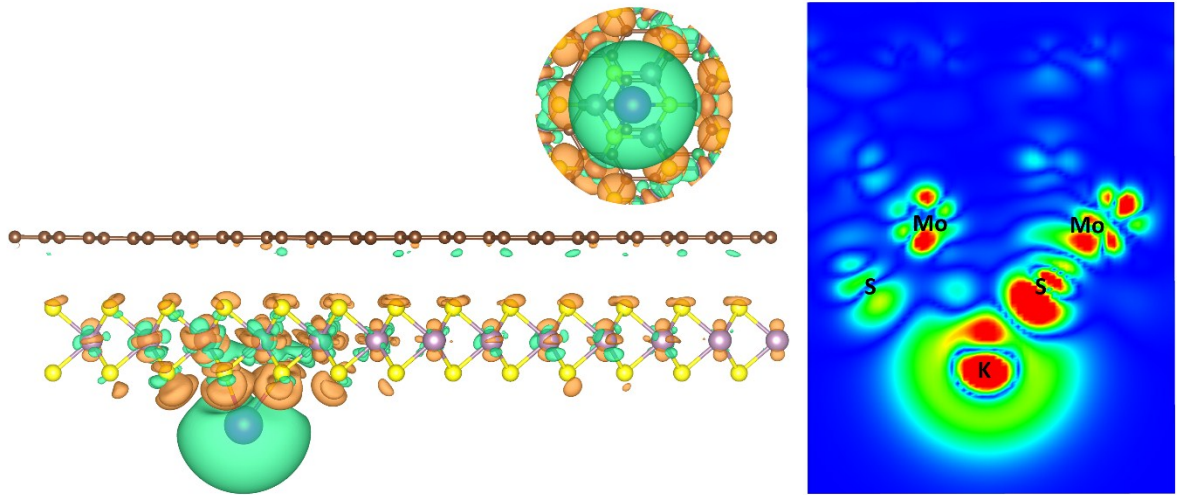


MoS₂ side:

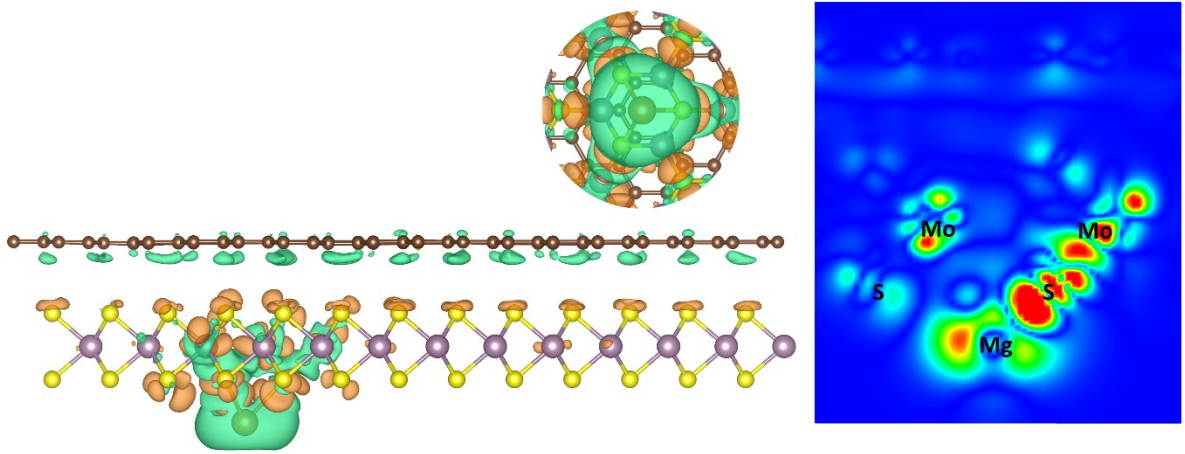
Al



K



Mg



Na

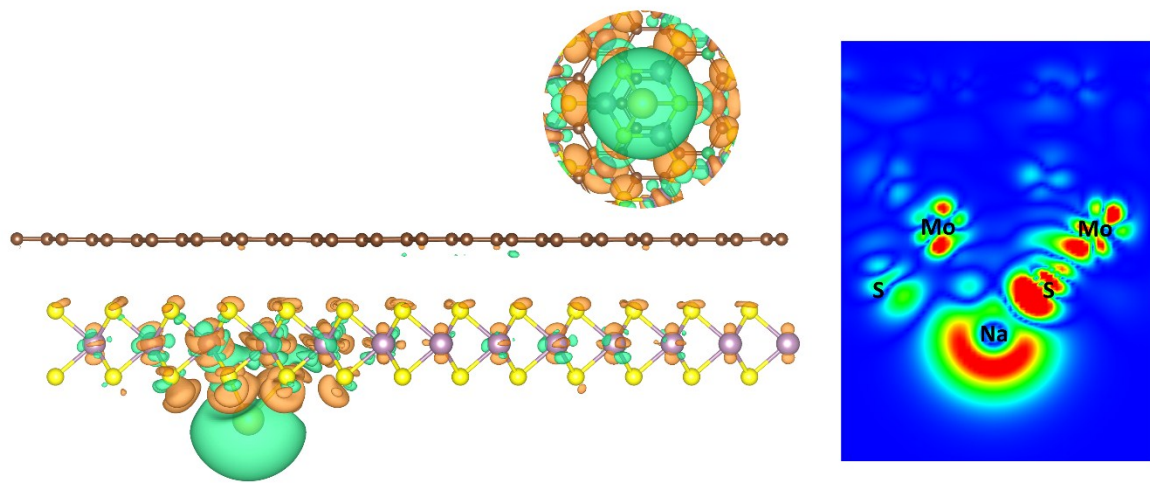


Fig.1 Vertical and horizontal (up view for situation (i) and (ii); bottom view for situation (iii)) views of charge density difference for adatoms in different regions. The (1, -1, 0) lattice plane is chosen for 2D mapping. The (1, -1, 0) lattice plane is chosen for 2D mapping. The isosurface is set to 0.0003. Orange and green represent electrons accumulation and depletion respectively.