Electronic Supplementary Information for

Graphene Buffered Galvanic Synthesis of Graphene-Metal Hybrids

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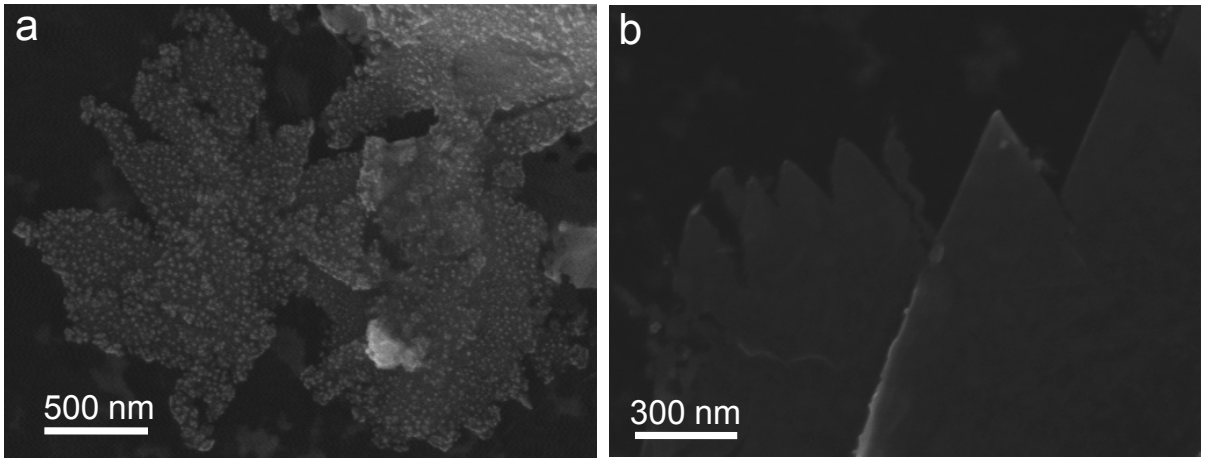
Simulation method

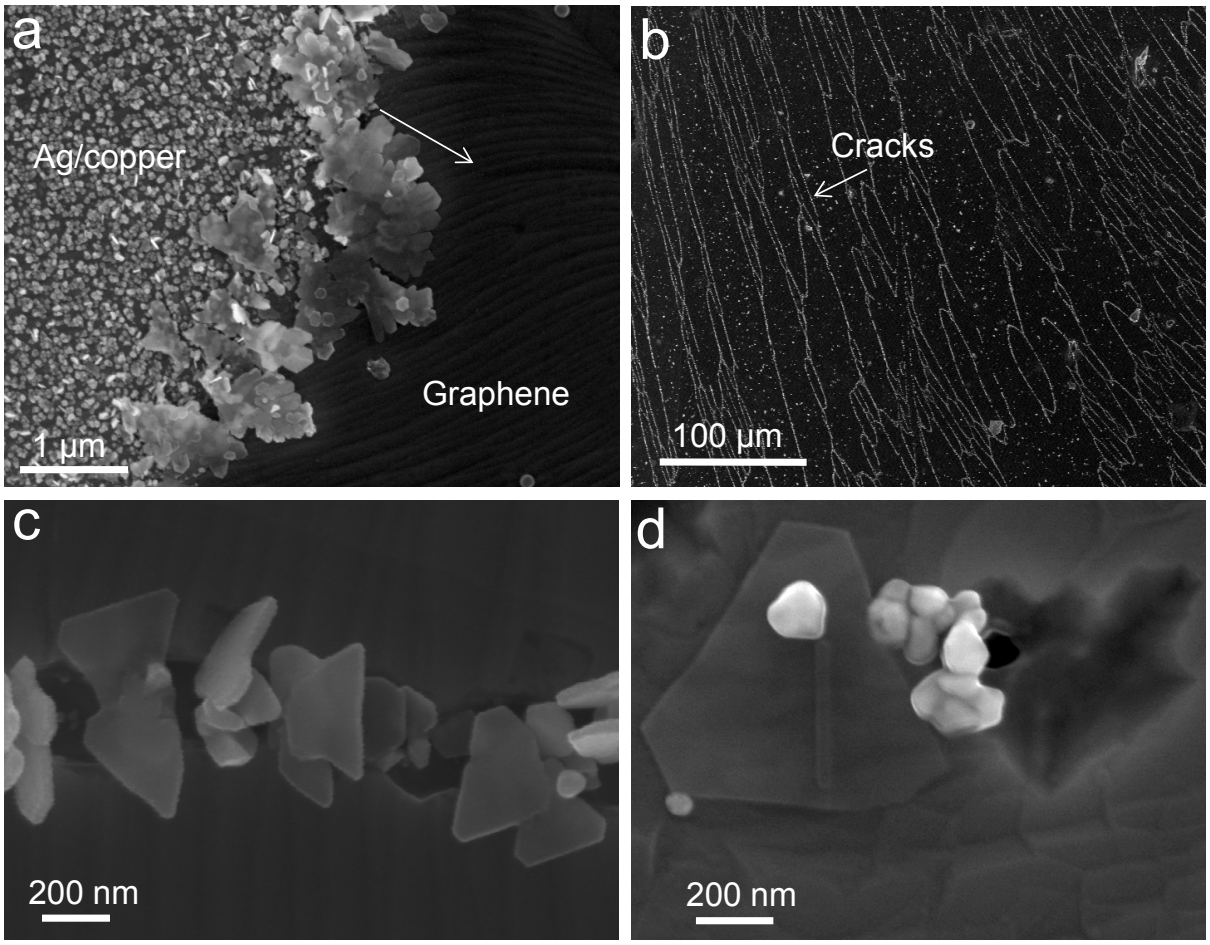
First-principles calculations are performed to obtain the binding energy between one silver atom and pristine or defected graphene sheets. The interface is investigated through a rectangular super-cell of 0.85 nm×0.93 nm. A vacuum layer of 2 nm is used in the direction normal to interface, representing the isolated boundary condition for the graphene sheet. For the binding site at the edge of graphene, the periodic boundary condition is removed and the extended graphene sheet becomes an isolated flake.

The structure and properties of this hybrid system are studied using plane-wave basis sets based density functional theory (DFT) methods. Local density approximation (LDA) is used for the exchange-correlation functional and projector augmented wave (PAW) potentials are used for ion-electron interaction. We use the Vienna Ab-inito Simulation Package (VASP) for the calculations. For all results presented, an energy cut-off of 300 eV is used for plane-wave basis sets. Monkhorst-Pack 4×4×1 grid points and the gamma point are used for Brillouin zone sampling for periodic and non-periodic system respectively. These settings have been verified to achieve a total energy convergence less than 1 meV/atom. For geometry relaxation, the force on atoms is converged below 0.01 eV/Å. All structures are initially optimized using a conjugated gradient method.

The binding energy between graphene and the silver atom is calculated as $E_b = E_{C\_Ag} - E_C - E_{Ag}$, where E_{C_Ag} is the total energy of the silver and graphene system, E_C is the energy of graphene sheet without binding silver atoms. E_{Ag} is the energy of an isolated silver atom.



(Fig. S1)



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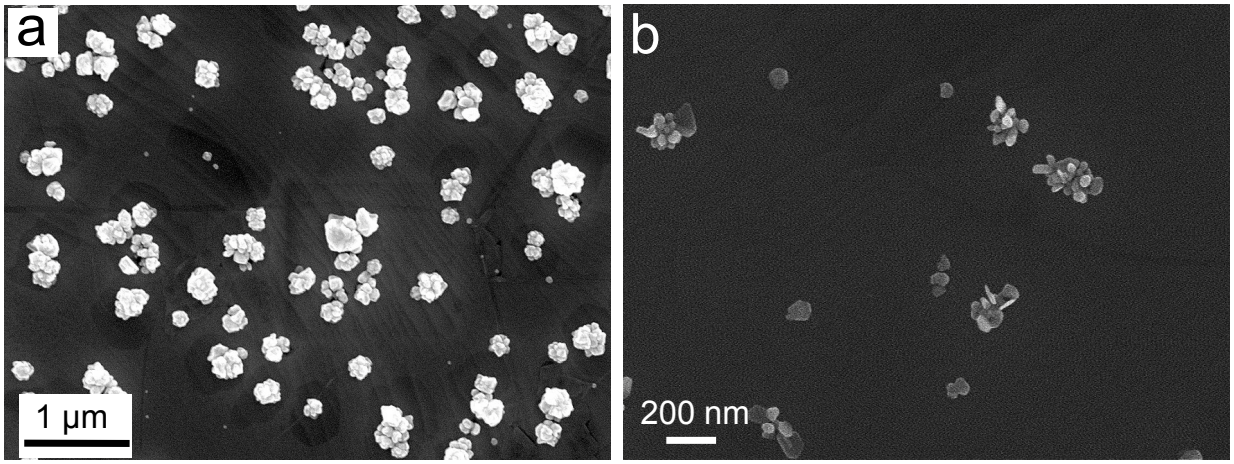

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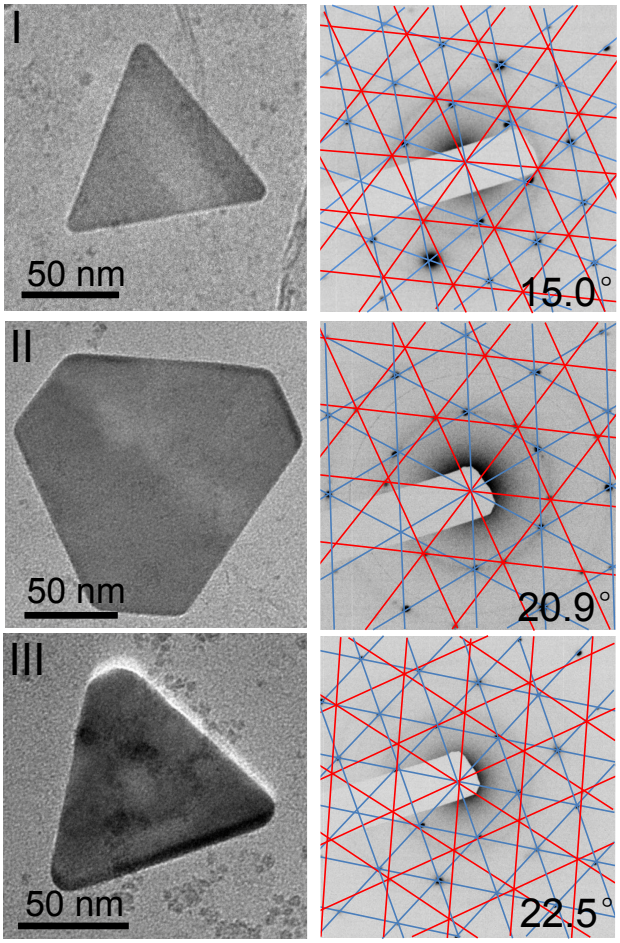

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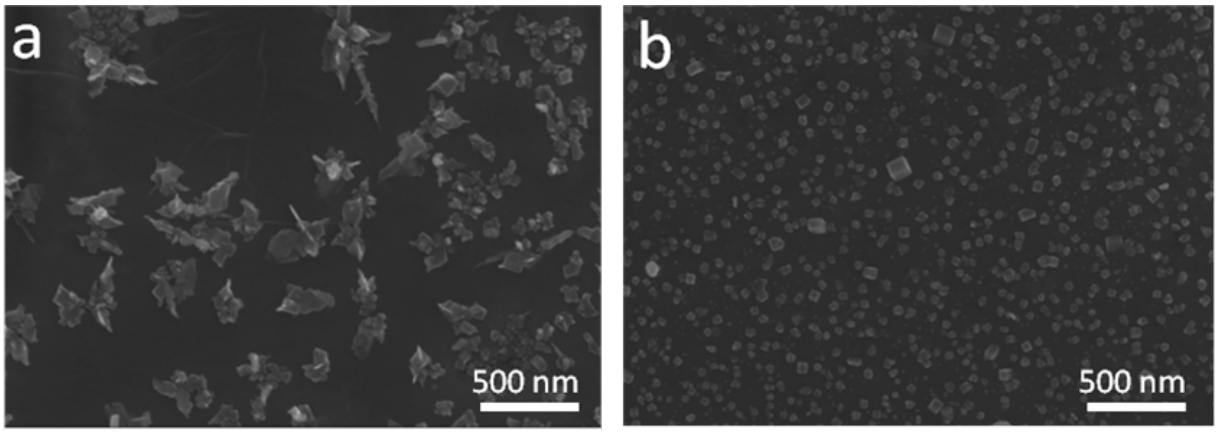
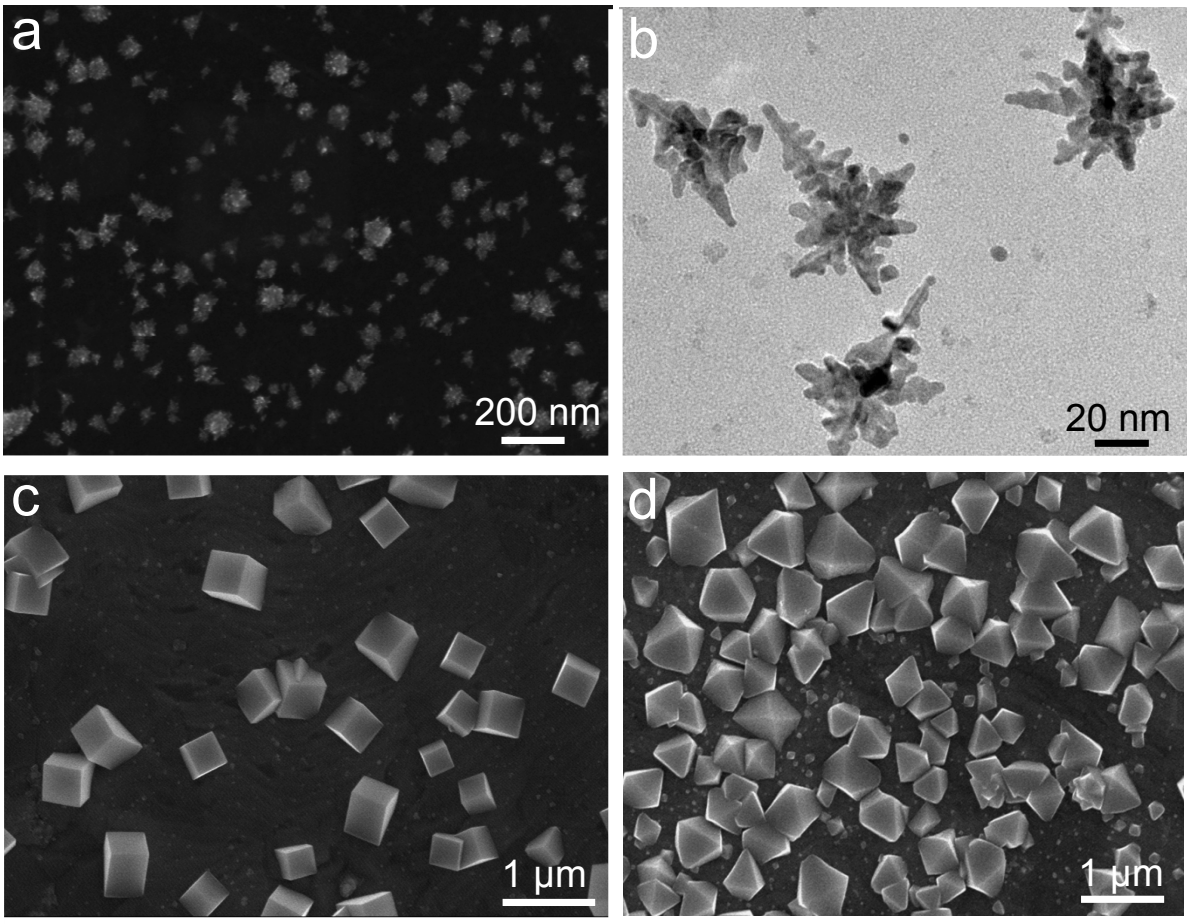


(Fig. S5)



(Fig. S5)