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ELECTRONIC EXCITATION SPECTRUM IN SILICENE GROWN ON SILVER

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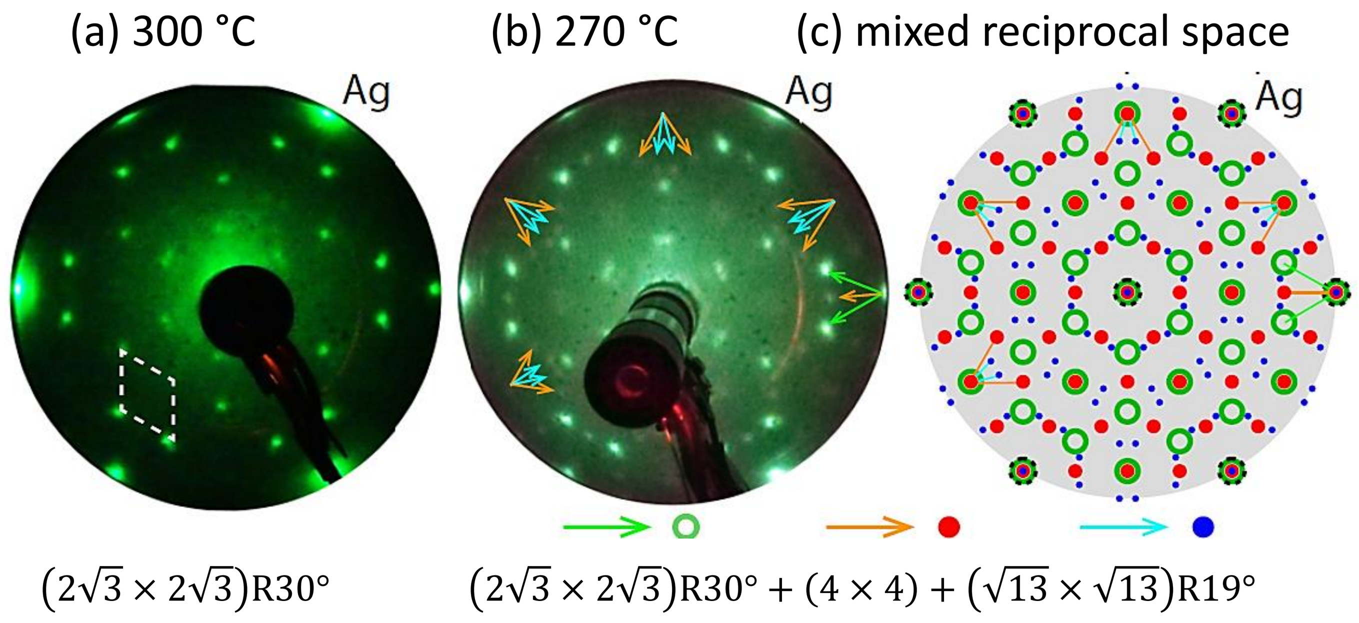
CONTEXT

Silicene, the two-dimensional allotrope of silicon, exists in a low-buckled honeycomb lattice, characterized by semimetallic electronic bands with graphene-like energy-momentum dispersions around the Fermi level (Dirac - cones electrons) [1,2].
Single layers of silicene are mostly synthesized by depositing silicon on top of silver, where, however, the different phases observed to date are strongly hybridized with the substrate that not only the Dirac cones, but also the whole valence and conduction states of ideal silicene appear to be quanched.

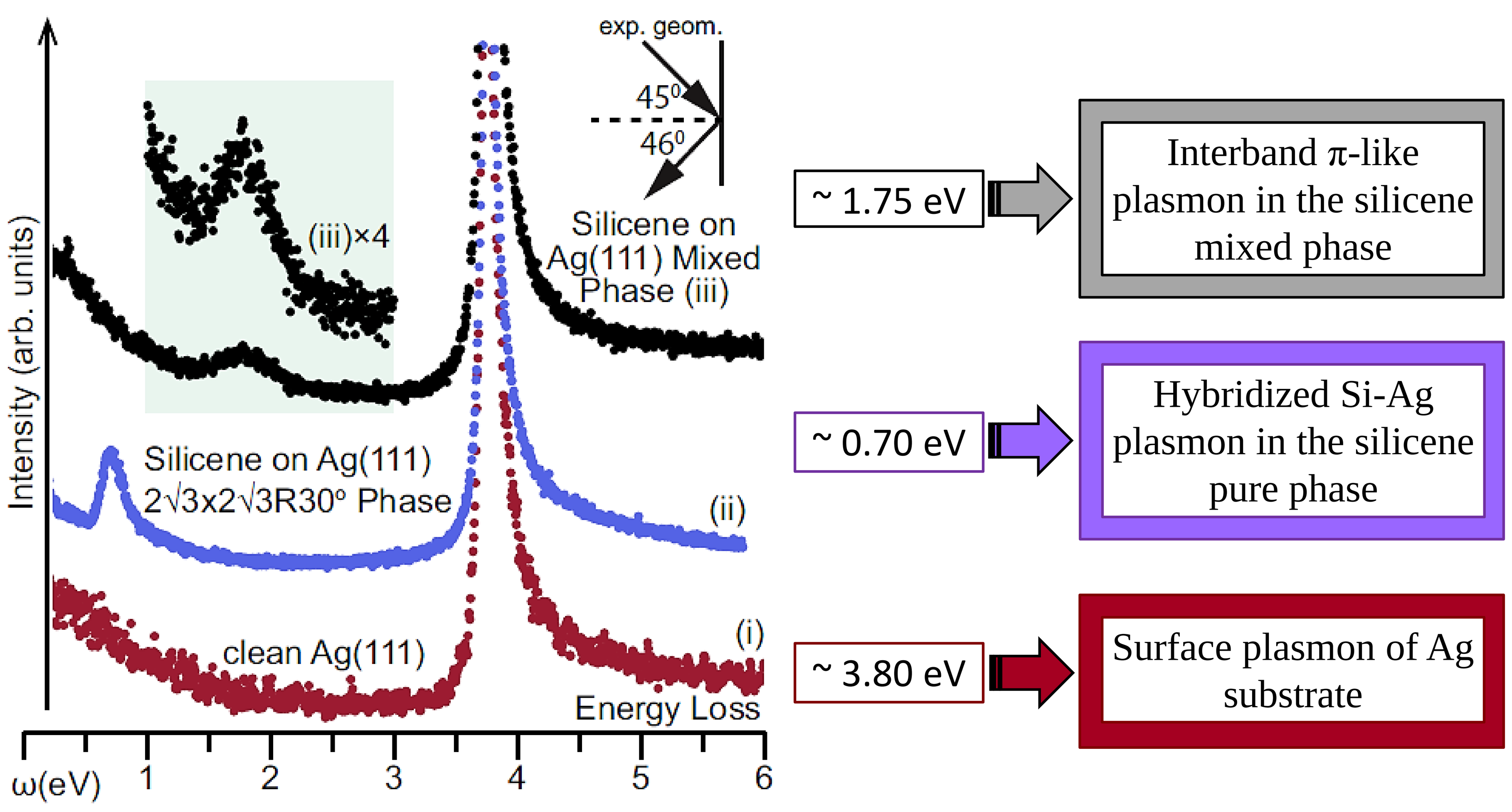
Here, we provide evidence that at least part of this semimetallic behavior is preserved by the coexistence of more silicene phases, epitaxially grown on Ag(111) [3].
In particular, by means of electron energy loss spectroscopy (EELS) and time-dependent density functional theory (TDDFT) we observe the low-energy plasmon in multiphase-silicene/Ag(111), prepared at controlled silicon coverage and growth temperature. We find that this mode survives the interaction with the substrate, being perfectly matched with the π-like plasmon of ideal silicene.

LOW-ENERGY ELECTRON DIFFRACTION (LEED)

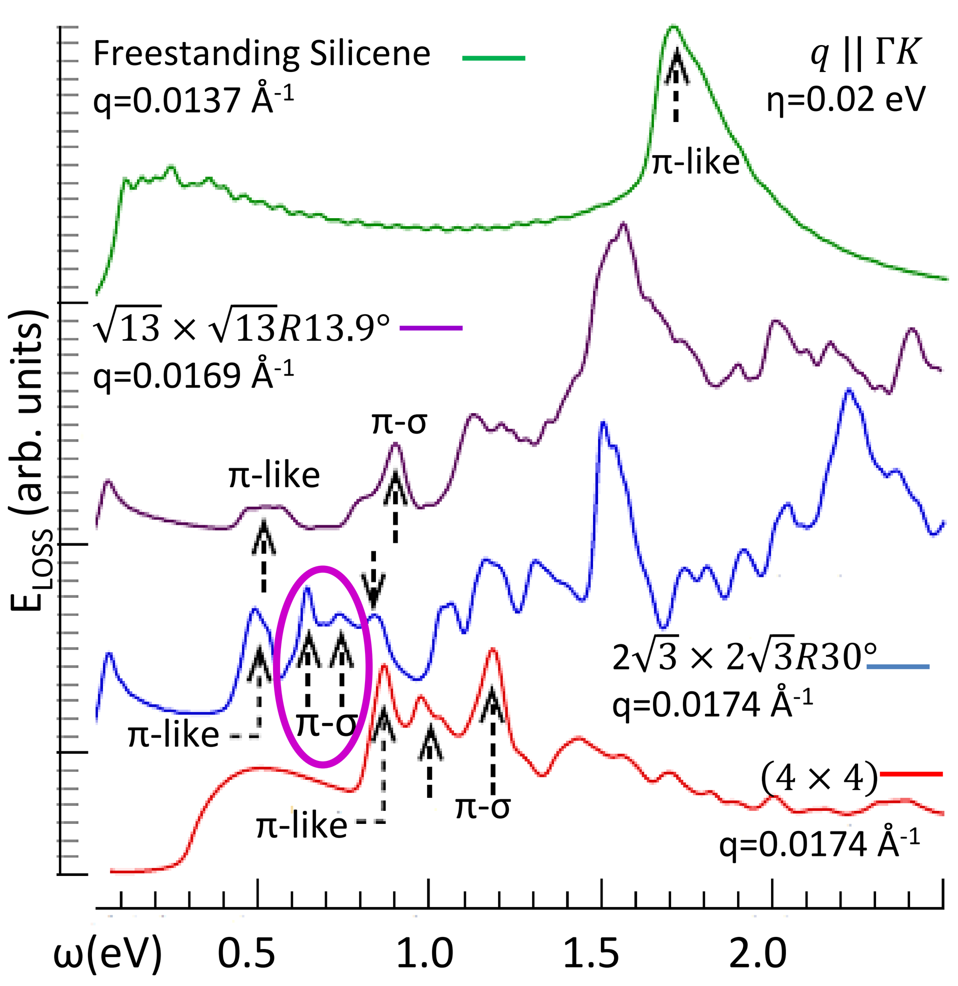


LEED patterns of (a) the $(2\sqrt{3}\times2\sqrt{3})$R30° phase and (b) the $(2\sqrt{3}\times2\sqrt{3})$R30° + (4×4) + $(\sqrt{13}\times\sqrt{13})$R19° phase of silicene on Ag(111).
The coexistence of multiple domains in (b) is attested by spots of different intensity, being consistent with the mixed reciprocal space representation in (c).

EXCITATION SPECTRUM PROBED BY EELS

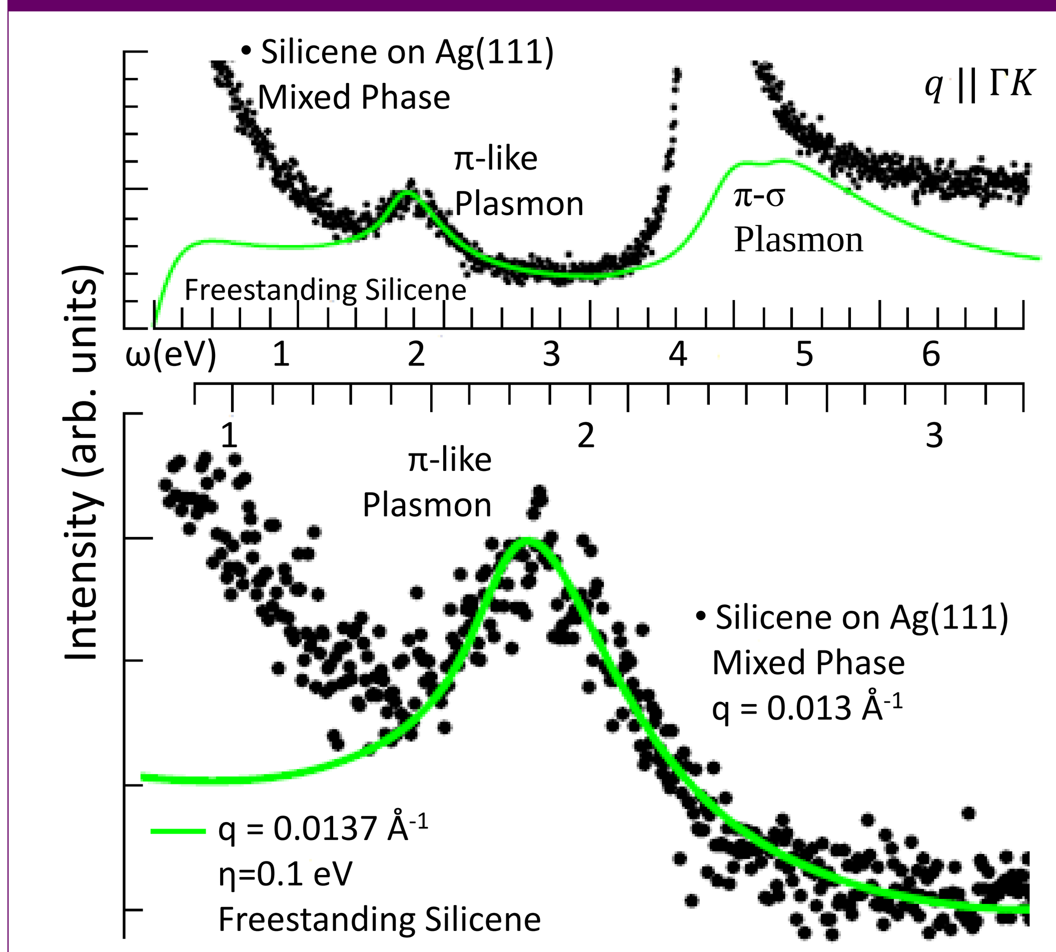


LOSS FUNCTIONS



- The experimental loss function of the pure phase $(2\sqrt{3}\times2\sqrt{3})$R30° shows a peak, matching with the $\pi-\sigma$ plasmon of the corresponding theoretical loss function.
- π-like mode is absent in each single pure phase.

SILICENE MIXED PHASE vs FREESTANDING SILICENE



The excellent agreement, at loss energies below 3 eV, leads to conclude that silicene mixed phase presents a dielectric response that matches expections for the π-like plasmon of ideal silicene.

CONCLUSIONS & PERSPECTIVES

- Silicene grown in a mixed phase on Ag(111) preserves at least part of the semimetallic character of its freestanding form, exhibiting an interband π-like plasmon.
- The progress on the epitaxial synthesis of pure, single phases of silicene on Ag(111), supported by DFT computations of their electronic properties, indicate that strong hybridization effects make it impractical to separate a silicene structure with a well-defined quasimetallic character. An experimental fingerprint of this phenomenon is the hybridized Si-Ag plasmon, discovered at low energy. Our proposal is then to shift the efforts of making silicene a feasiblle two-dimensional nanomaterial beyond graphene on the epitaxial growth of silicene in mixed domains.

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