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Supporting Information for

Topological quantum catalyst: the case of two-dimensional traversing nodal line states associated with high catalytic performance for hydrogen evolution reaction

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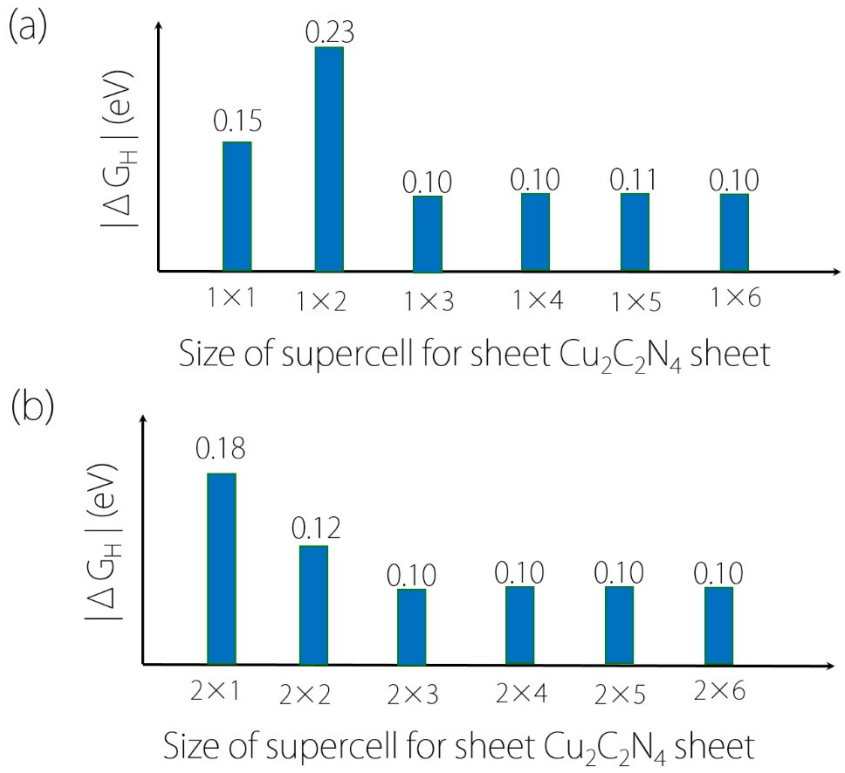
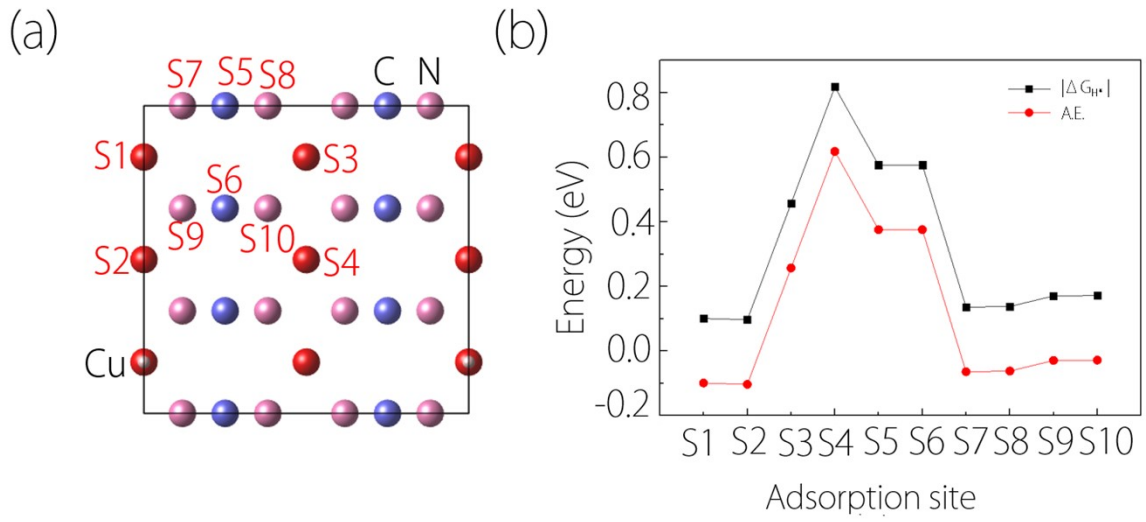
I. Adsorption model

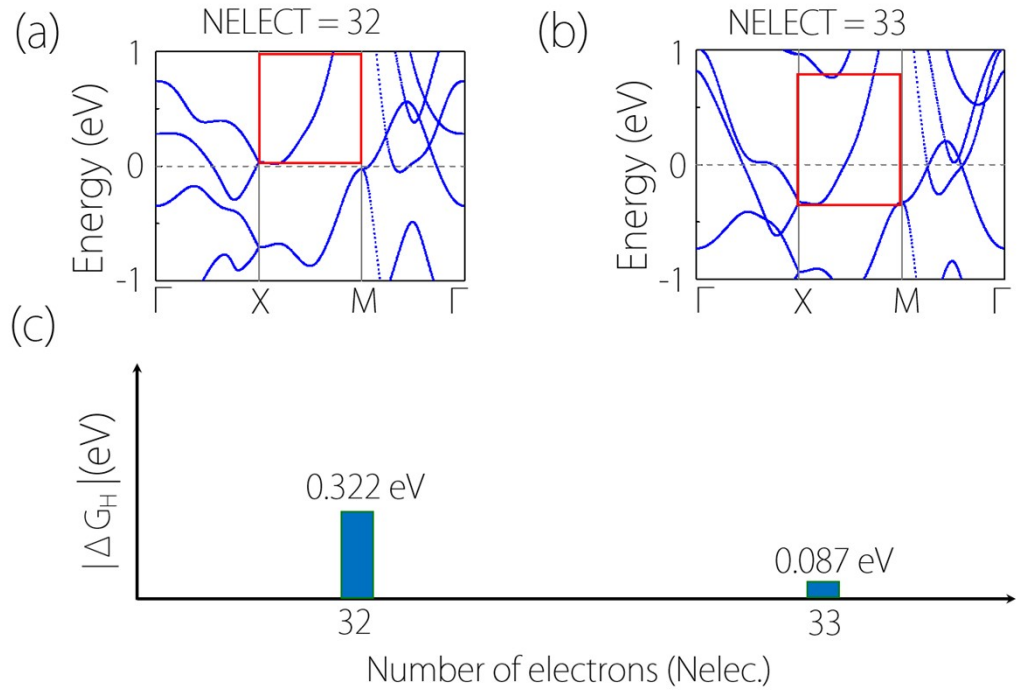


FigS1 Comparison of $|\Delta G_{H^*}|$ for $Cu_2C_2N_4$ sheet under different sizes of supercell.



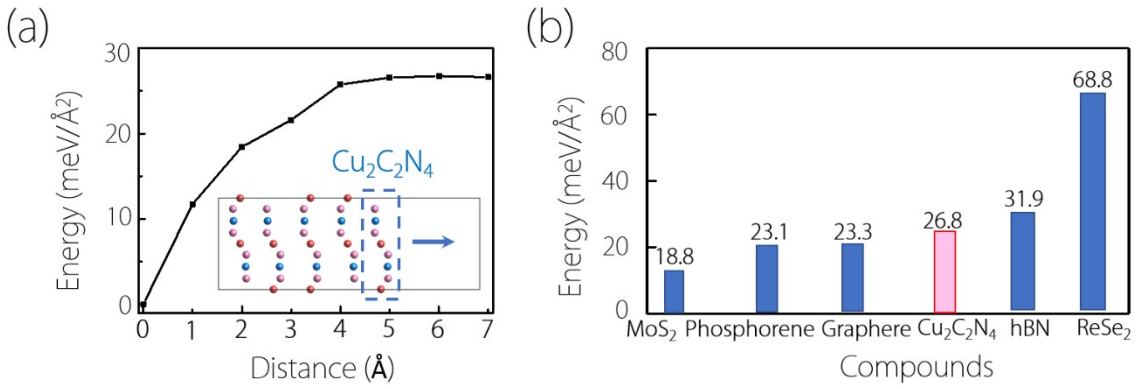
FigS2 (a) The selected adsorption sites (denoted as S1-S10) in the 1×3 supercell of $Cu_2C_2N_4$ sheet. (b) comparison of $|\Delta G_{H^*}|$ and adsorption energy (A.E.) among different adsorption sites.

II. Electronic structure and ΔG_{H^*} in 2D TiZn



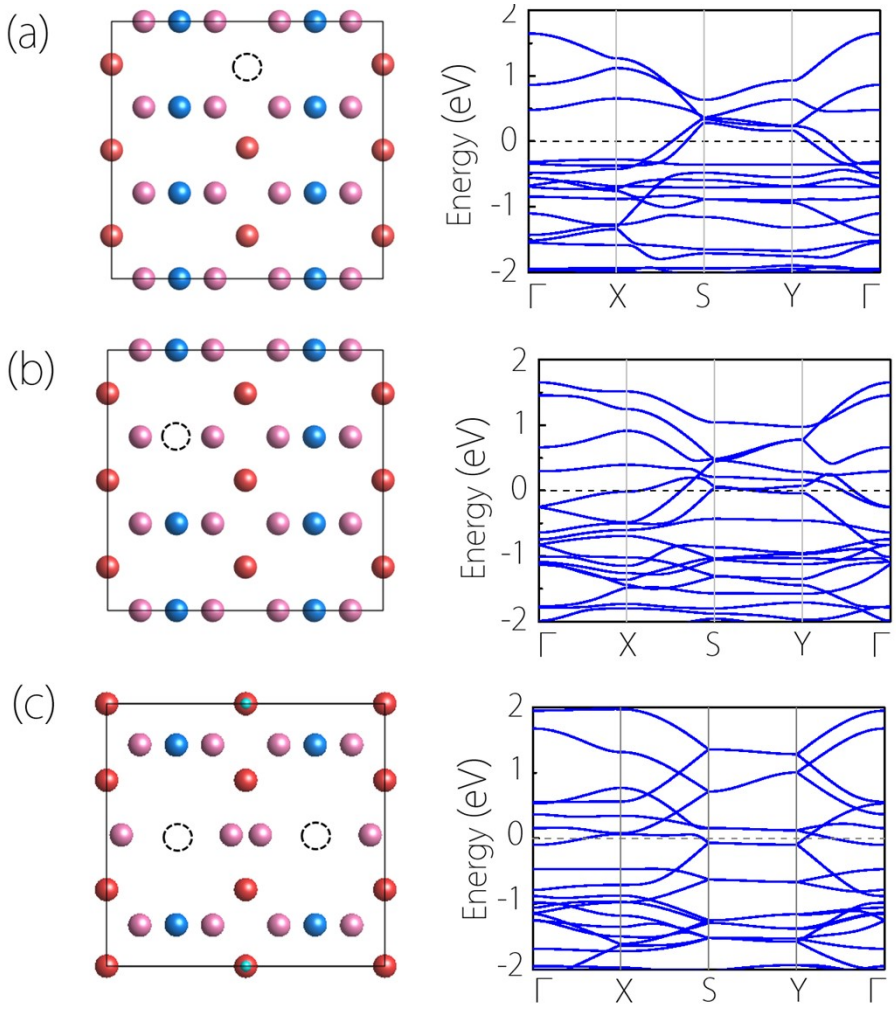
FigS3 Electronic band structure for TiZn (a) without and (b) with one electron doping. The framed region in the band structure shows the position of open nodal line. (c) Comparison of $|\Delta G_{H^*}|$ for TiZn without (Nelec.= 32) and with electron doping (Nelec.= 33).

III. Exfoliation feasibility of $Cu_2C_2N_4$ sheet



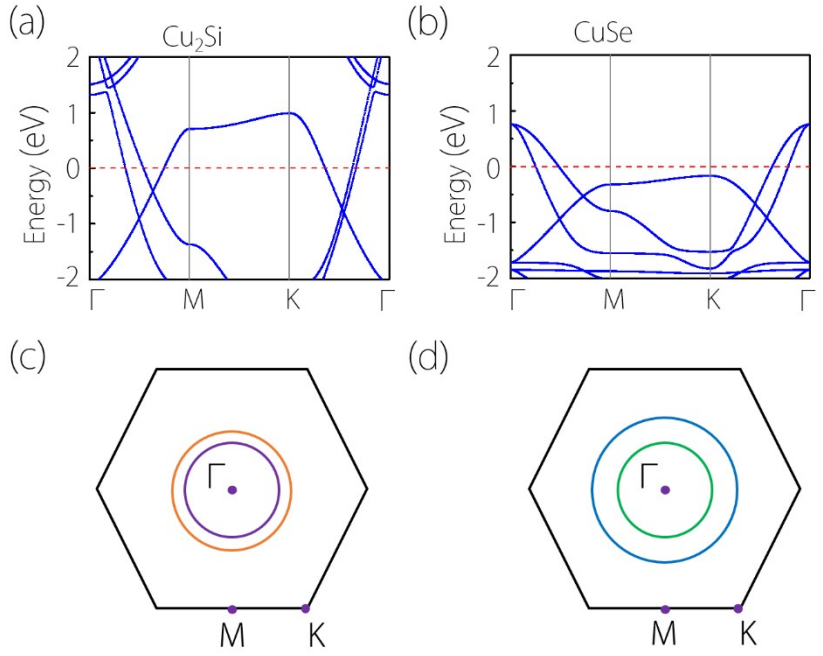
FigS4 (a) The model and results for exfoliation energy calculation of $Cu_2C_2N_4$ sheet. (b) Comparison of exfoliation energy in $Cu_2C_2N_4$ sheet and other typical monolayers. Some data in (b) are taken from references [N*ano Lett. 18, 5, 2759–2765 (2018)*; *ACS Appl. Mater. Interfaces 8, 5385−5392 (2016)*].

IV. Defect model and band structure

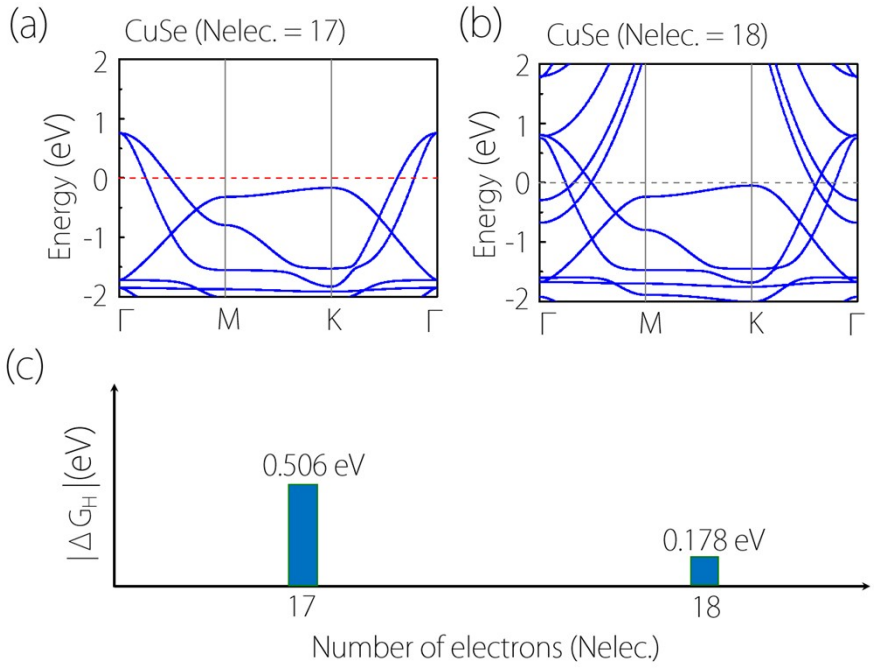


FigS5 (a) Crystal structure and electronic band structure of $Cu_2C_2N_4$ sheet with one Cu defect. (b) and (c) are similar with (a) but for the cases with one C defect and two C defects. In (a) and (b), the S_{2y} symmetry is broken, and the nodal lines do not occur. In (c), the S_{2y} symmetry and the nodal line in the S-Y path is preserved.

IV. Band structure and ΔG_{H^*} for Cu2Si and CuSe



FigS6 (a) Electronic band structure of Cu_2Si monolayer. (b) Electronic band structure of CuSe monolayer. (c) Illustration of two closed nodal lines in Cu_2Si monolayer. (d) Illustration of two closed nodal lines in CuSe monolayer.



FigS7 Electronic band structure of CuSe (a) without and (b) with one electron doping. (c)) Comparison of ΔG_{H^*} of CuSe before and after electron doping.