

Supporting Information (SI) for

Semi-Dirac Semimetal in Silicene Oxide

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1. The convergence test for energy cutoff

We have tested the total energy per atom of the atomic structures as a function of energy cutoff, as displayed below, for all oxides, sulfides and selenides. According to our test, we chose 550 eV, 350 eV and 300 eV as energy cutoff for oxides, sulfides and selenides, respectively.

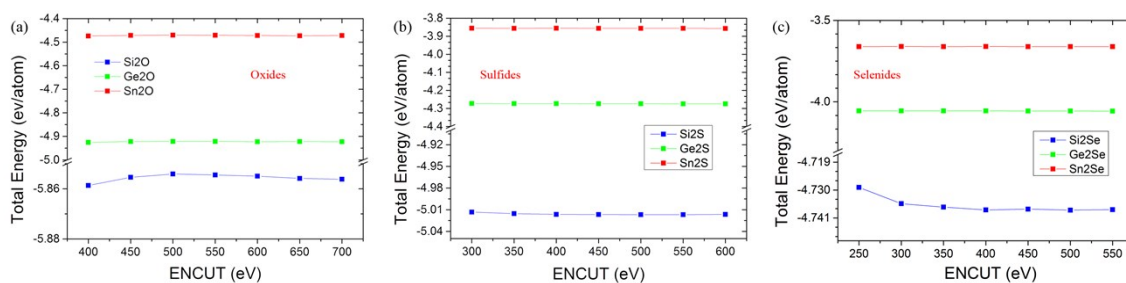


Figure S1. (a)-(c) The total energy per atom as a function of energy cutoff for oxides, sulfides and selenides on silicene, germanene and stanene, respectively.

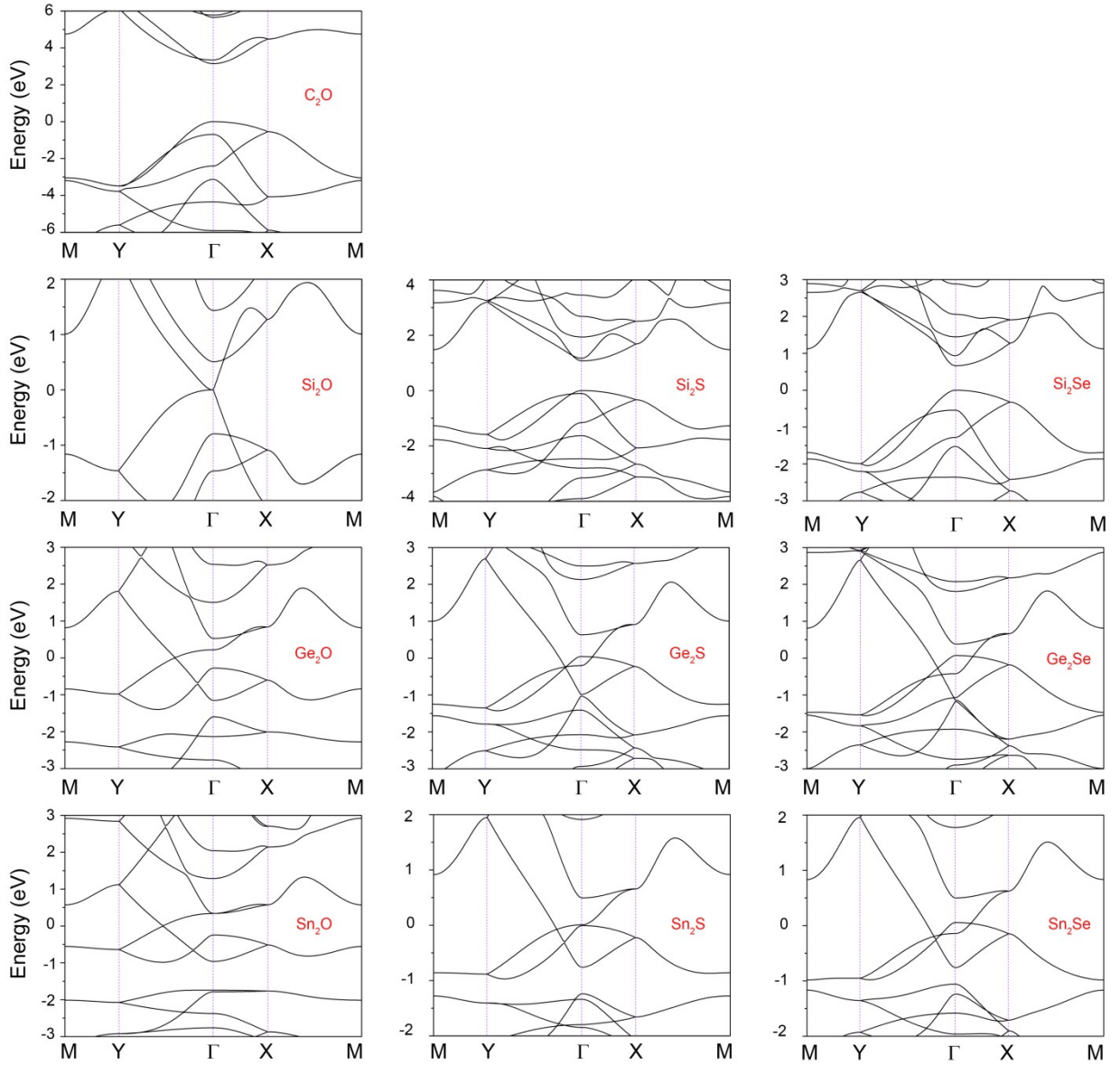


Figure S2. The band structures of honeycomb materials modified by group-VI elements. The atomic structures are similar to that in Figure 2a in the main text. The first row shows the results for graphene-based materials, where only graphene oxide was found stable and the sulfide and selenide are not. The second, third and fourth rows show the results for modified silicene, germanene and stanene, respectively.

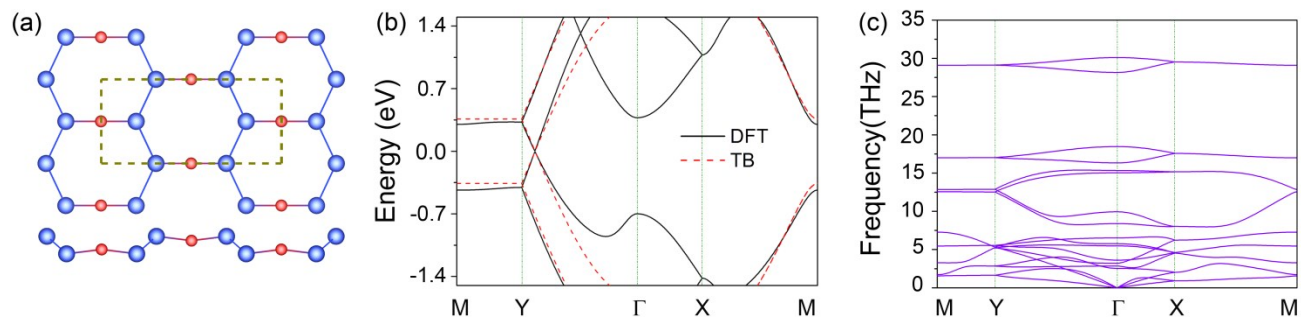


Figure S3. (a) Top view and side view of Si₂O-II. The dashed rectangle represents the unit cell. (b) Band structure of Si₂O-II from DFT and TB calculations. In TB calculation, $t_1 = 1.0$ eV and $t_2 = 0.36$ eV. (c) Phonon spectrum of Si₂O-II.

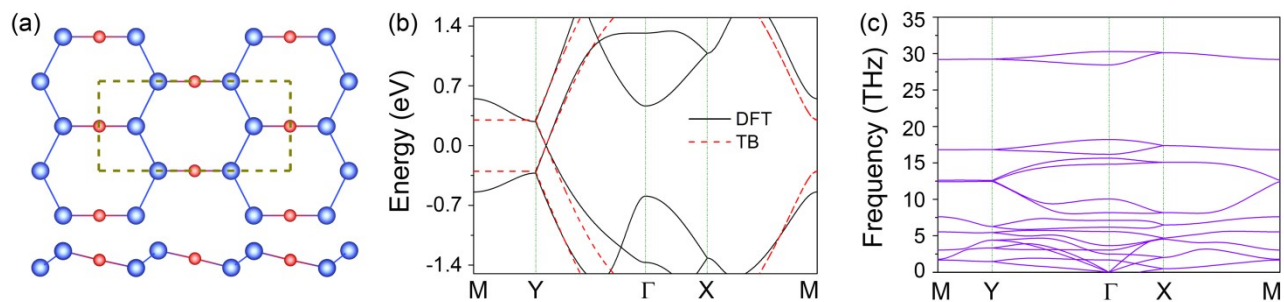


Figure S4. (a) Top view and side view of Si₂O-III. The dashed rectangle represents the unit cell. (b) Band structure of Si₂O-III from DFT and TB calculations. In TB calculation, $t_1 = 1.0$ eV and $t_2 = 0.30$ eV. (c) Phonon spectrum of Si₂O-III.