Supporting Information for 'A two-dimensional quinazoline based covalent organic framework with a suitable direct gap and superior optical absorption for photovoltaic applications'

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Supporting Figures

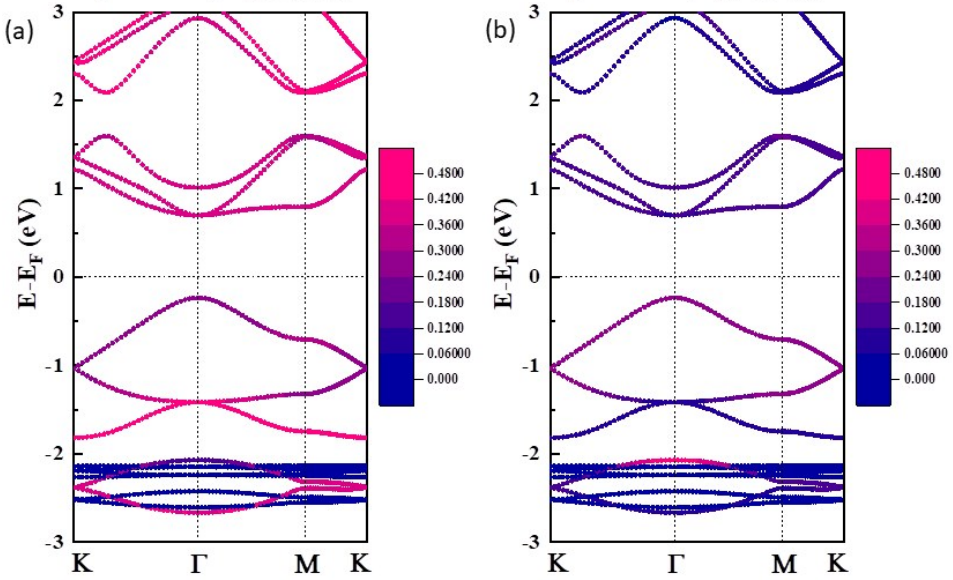

Fig. S1. Orbital projected band structures p_z orbitals of carbon (a) and nitrogen (b) of Q-COF monolayer calculated with the PBE functional, respectively.

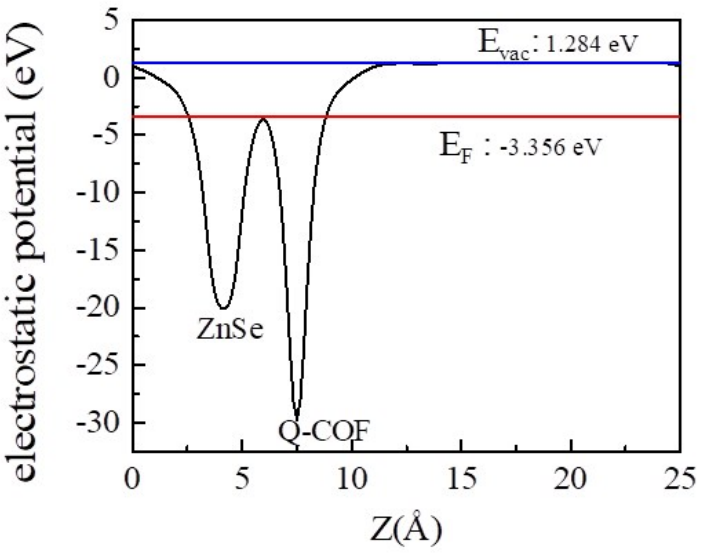

Fig. S2. Calculated electrostatic potential for Q-COF/ZnSe heterojunction. The red and blue lines denote the Fermi level and the vacuum energy level, respectively.

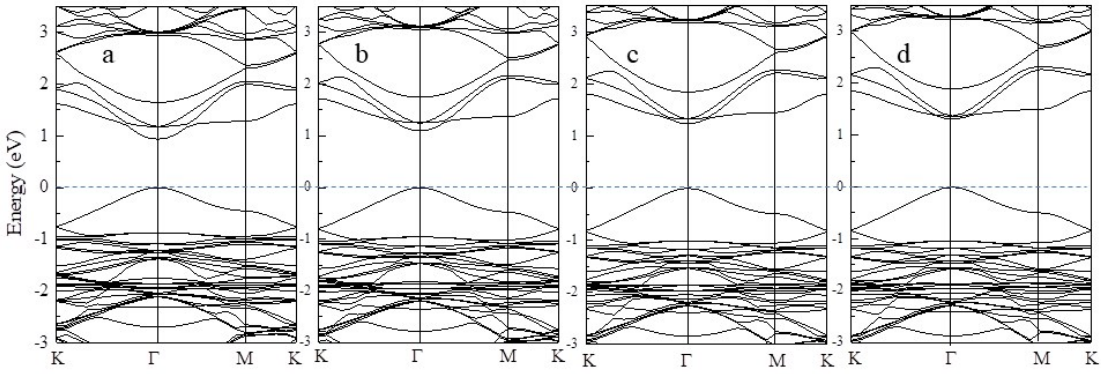

Fig. S3. Band structures of Q-COF/ZnSe heterojunction under compression strain: (a) 0; (b) -1.0%; (c) -1.8%; (d) -2.6%. The Fermi level was set to zero, as shown by the dashed line.