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Supplementary Materials

Highly Efficient $CuInSe_2$ Sensitized TiO_2 Nanotube Films for Photocathodic Protection of 316 Stainless Steel

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Computational methods

All calculations were carried out using the Vienna Ab-initio Simulation Package (Vasp). The Perdew-Burke-Ernzerhof (PBE) formula of the generalized gradient approximation (GGA) was adopted to describe the exchange-correlation effects. All calculations were carried out with a set cutoff energy (400 eV) and self-consistent convergence accuracy (1×10^{-5} eV). The k-point meshes were set as $3 \times 1 \times 1$ of the TiO_2 and $CuInSe_2$. The convergence criterion of the force between atoms and the maximum displacement are 0.03 eV/A and 0.001 A, respectively.