First-principle investigation 3,4-ethylenedioxythiophene molecule adsorption on Cu(110)-(2 × 1)O surface

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Highlights

- The most favorable adsorbing geometry is the thiophene ring of EDOT parallel to the Cu and molecule upright.
- Both dimer and tetramer can form under suitable EDOT coverage.
- The binding mechanism of EDOT on substrate is clarified.
- The dimer and tetramer are neither cis synthesized recently nor traditional anti structure.