



# Dynamics of Molecular Adsorption of CO on Cu(110)

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## Abstract

# **1 Introduction**

## **2 Methodology**

### **2.1 DFT Calculations**

### **2.2 NN PES parametrization and accuracy tests**

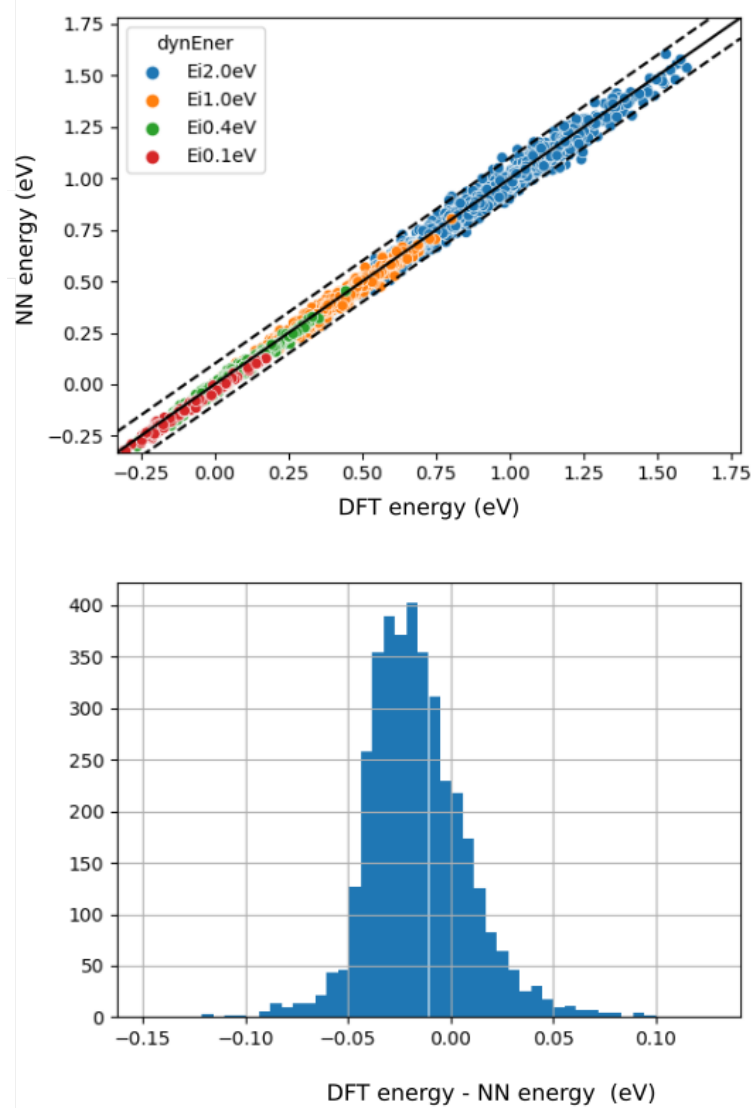


Figure 1: ....

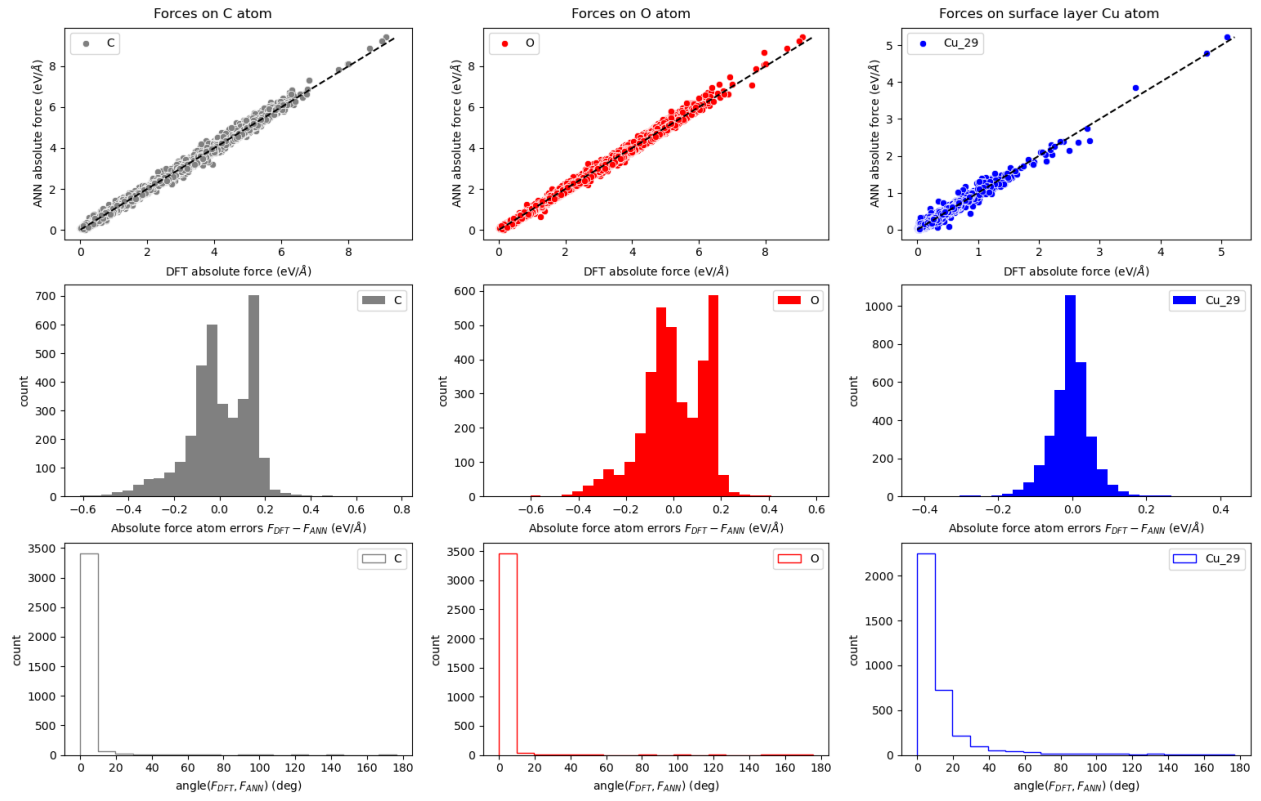


Figure 2: ....

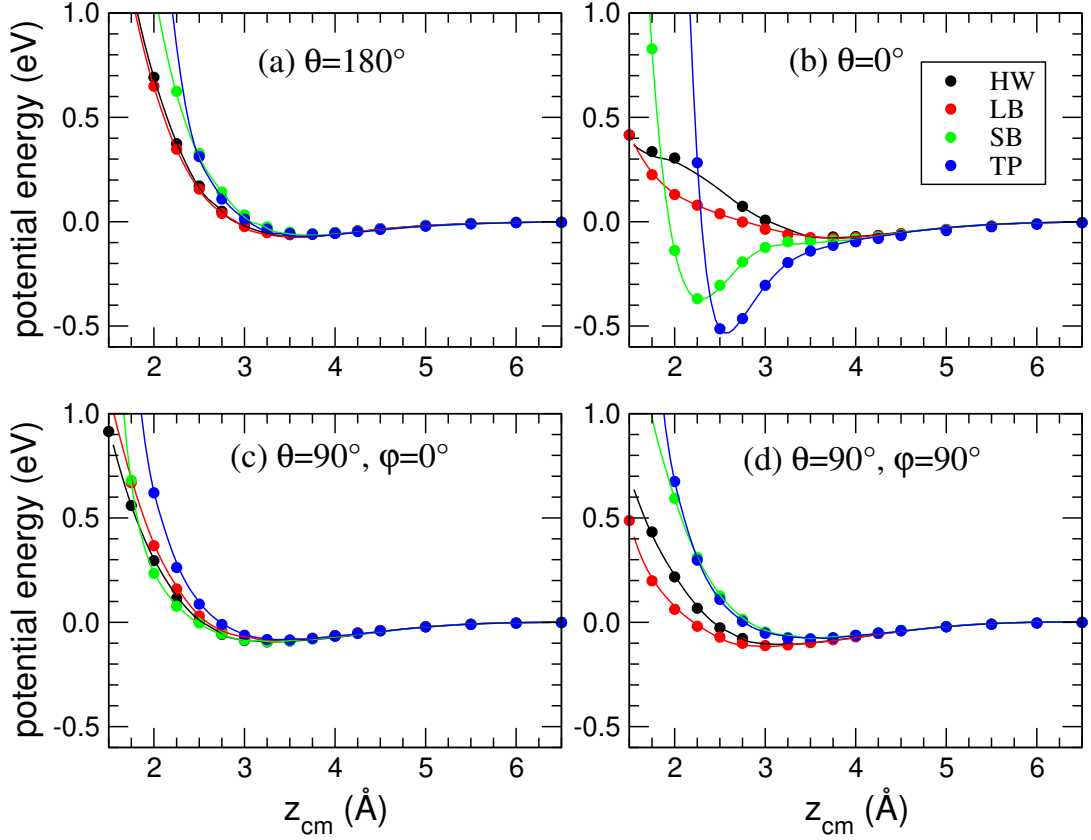


Figure 3: Comparison of DFT total energies (full circles) and PES-ANN results (full lines) for CO/Cu(110) on four high symmetry surface sites: top (TP), blue; short-bridge (SB), green; long-bridge (LB), red; four-fold hollow (HW), black, as a function of the z coordinate of the molecular center of mass,  $z_{cm}$ .  $z=0$  corresponds to the plane of the Cu atoms in the outermost surface layer. (a) CO perpendicular to the surface with O down, (b) CO perpendicular to the surface with C down, (c) CO parallel to the surface and parallel to the the  $[-110]$  direction (x axis), (d) CO parallel to the surface and parallel to the the  $[-001]$  direction (y axis).

### 3 Results and discussions

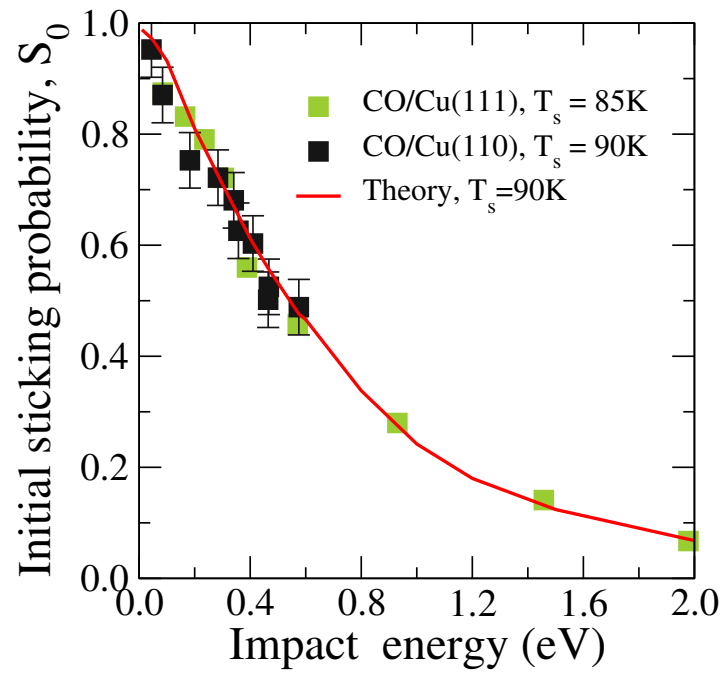


Figure 4: ....



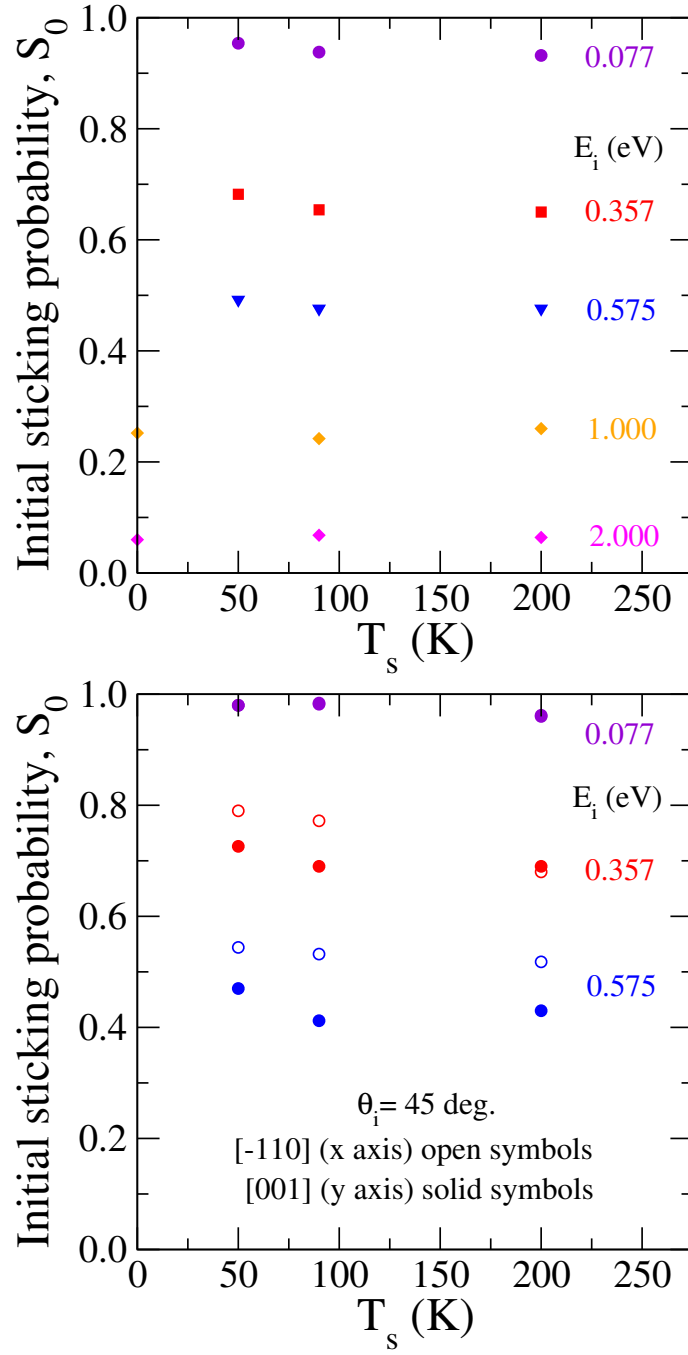


Figure 5: ....

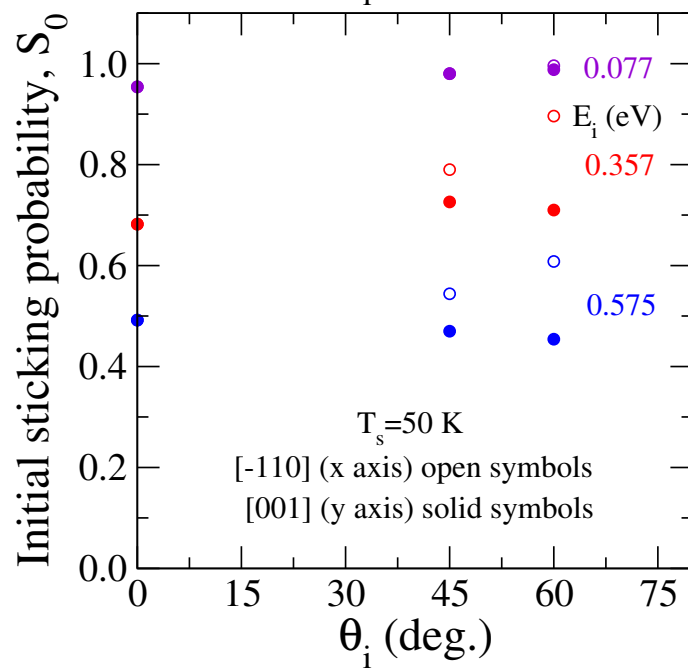
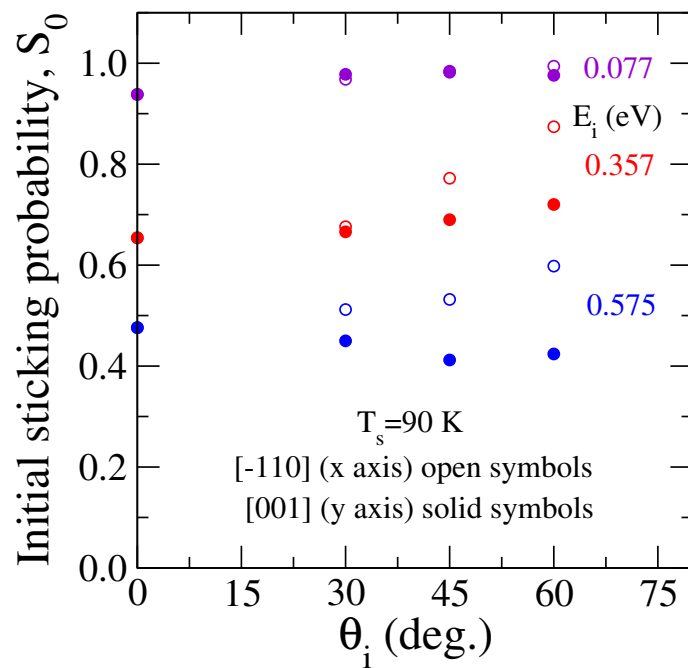


Figure 6: ...

## 4 Conclusions

## 5 Supporting Information

Details about the PES-ANN developed and used in the present work.

## 6 Acknowledgments

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## 7 Author Contributions

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All the authors participated in the discussion of the results, and writing and/or revision of the manuscript.

## 8 Conflicts of Interest: None

## Graphical TOC Entry

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