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The role of defects and phonons in O_2 adsorption on Cu(100)
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We present the results of an extensive *ab initio* study for O_2 adsorption on the Cu(100) surface. The calculated potential energy surfaces and first principles molecular dynamics trajectories reveal that on the clean surface without defects the dissociation probablility is low at small translational energies of the incoming molecule wheras at higher energies the molecules dissociate directly without a barrier. Of the different defects, steps turn out to be less reactive than expected and adatoms rather lower than enhance the reactivity. In contrast, vacancies act as dissociative centers, which locally enhance the reactivity. This result is in agreement with the molecular beam surface scattering experiments which show an increase at the oxygen sticking probability at low energies. We also discuss the role of phonons in O_2 dissociation, showing that the open space involved at certain phonon modes lowers the dissociation barrier, an effect analogous to the vacancy induced dissociation. Our results clearly demonstrate the importance of including both defects and surface dynamics in a realistic description of the adsorption process.

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