

I. SUPPLEMENTARY MATERIAL

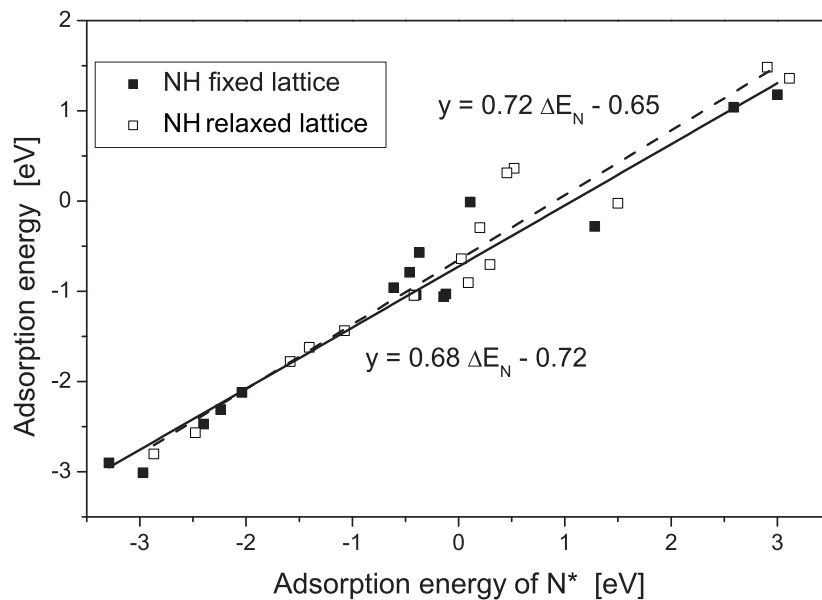


FIG. 1. The scaling relations of the NH specie on both the bulk M12 and relaxed M12.

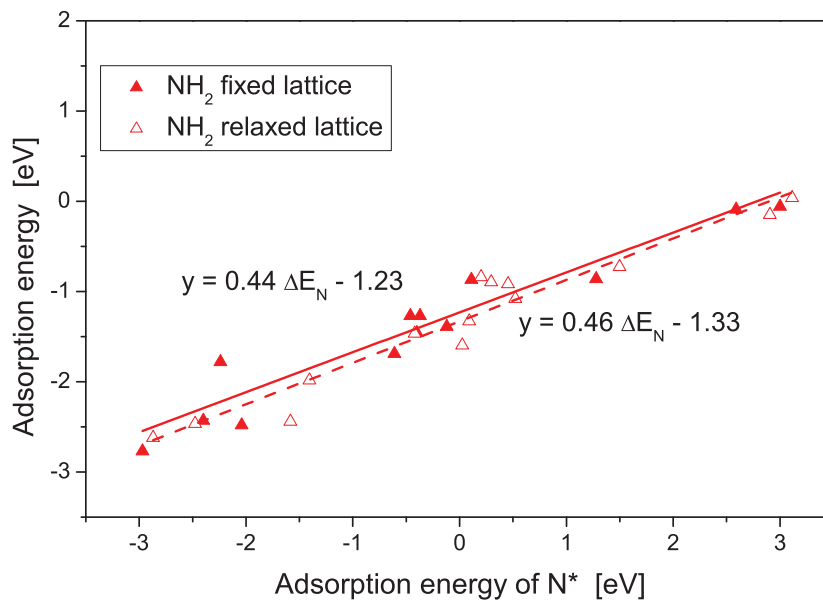


FIG. 2. The scaling relations of the NH₂ specie on both the bulk M12 and relaxed M12.

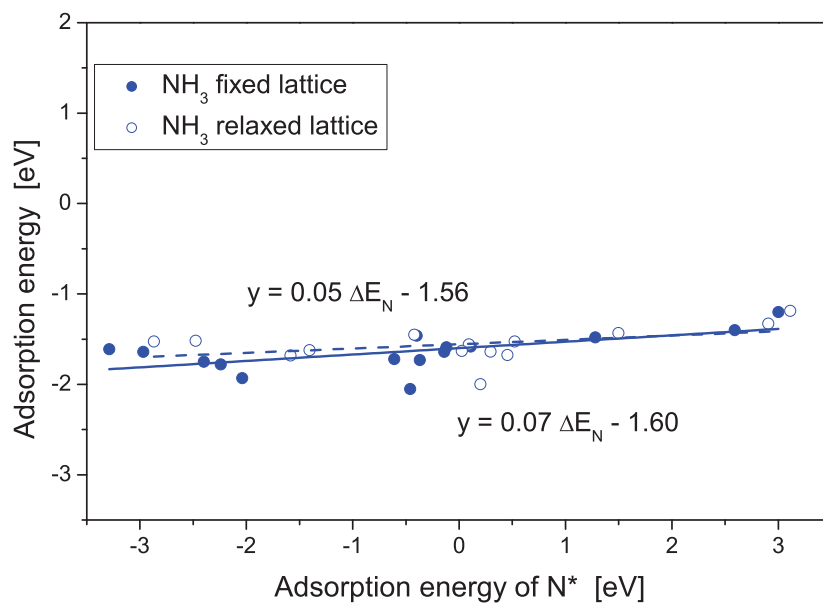


FIG. 3. The scaling relation of the NH_3 specie both the bulk M12 and relaxed M12.

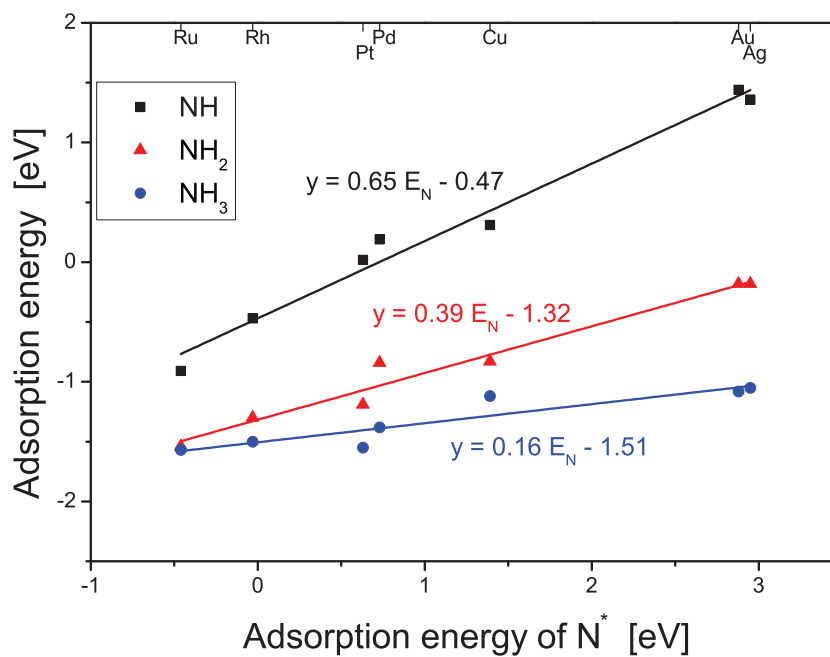


FIG. 4. The scaling relations for NH_x species on the stepped $\text{fcc}(211)$ surface consisting of transition metals.

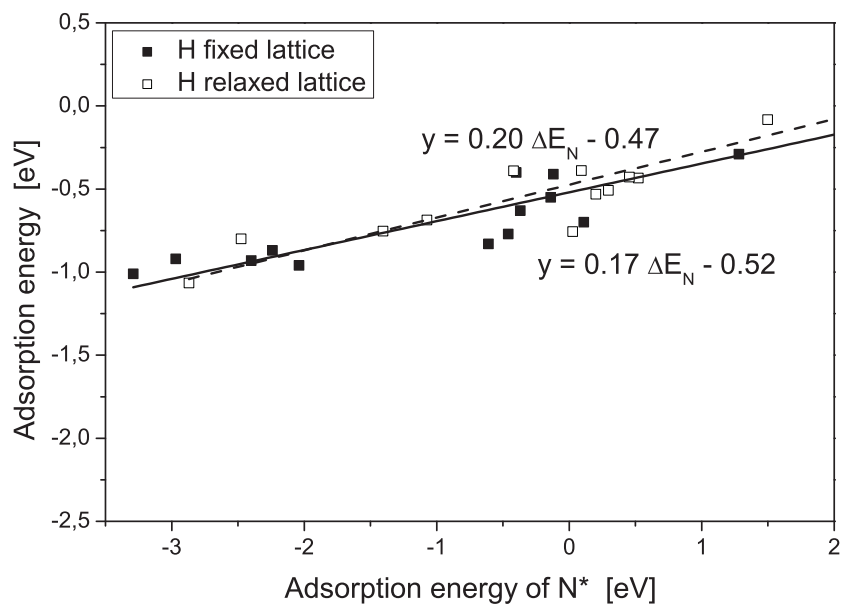


FIG. 5. The scaling relations of H on both the bulk M12 and relaxed M12.

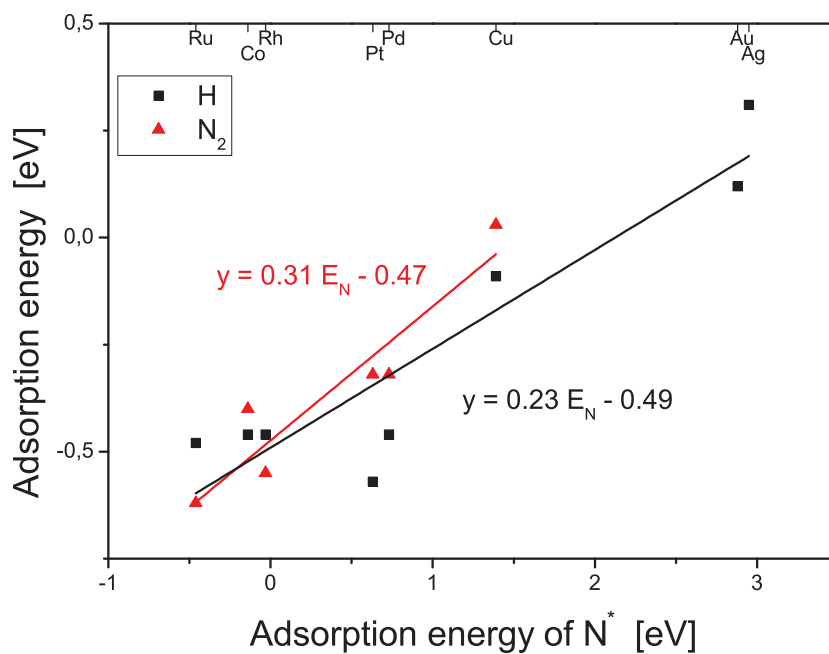


FIG. 6. The scaling relations of N₂ and H species on the stepped fcc(211) surface consisting of transition metals.

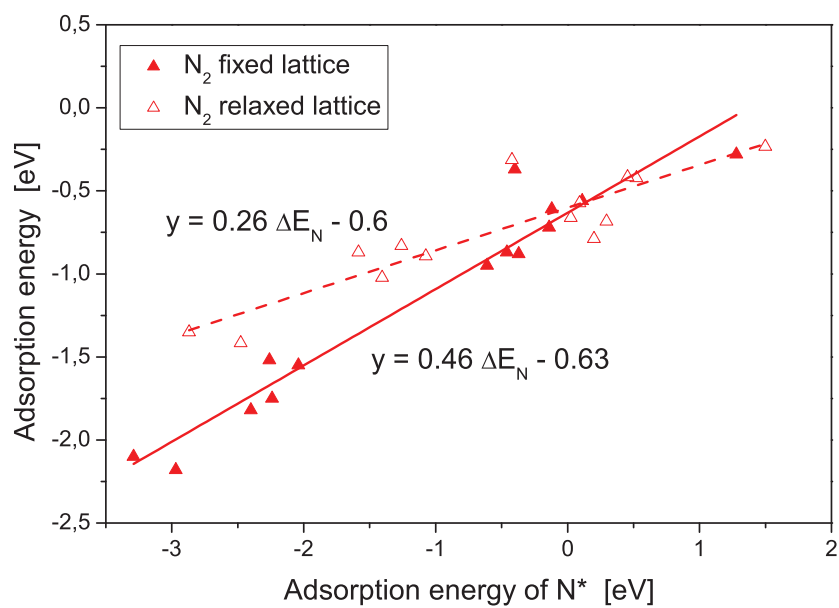


FIG. 7. The scaling relations of the N_2 specie on both the bulk M12 and relaxed M12.

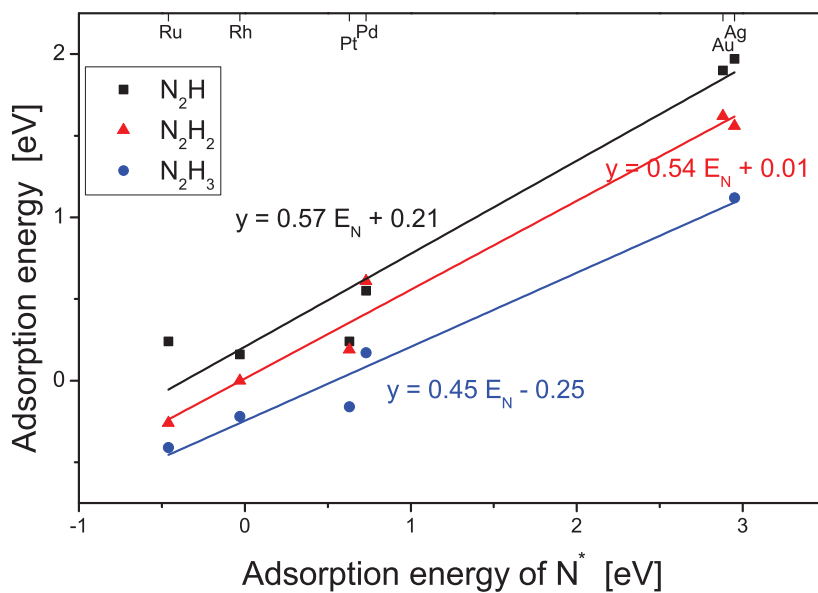


FIG. 8. The scaling relations for N_2H_x species on the stepped $fcc(211)$ surface consisting of transition metals.

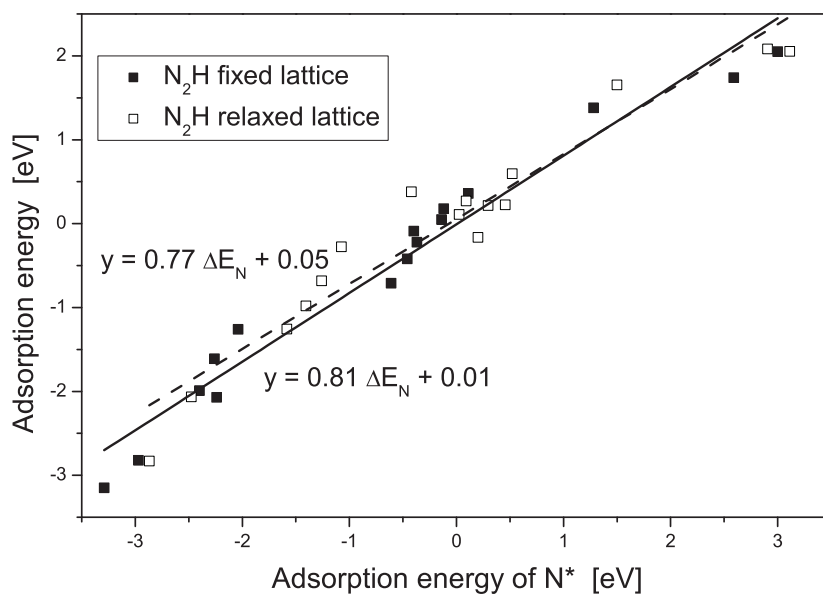


FIG. 9. The scaling relations of the N_2H specie on both the bulk M12 and relaxed M12.

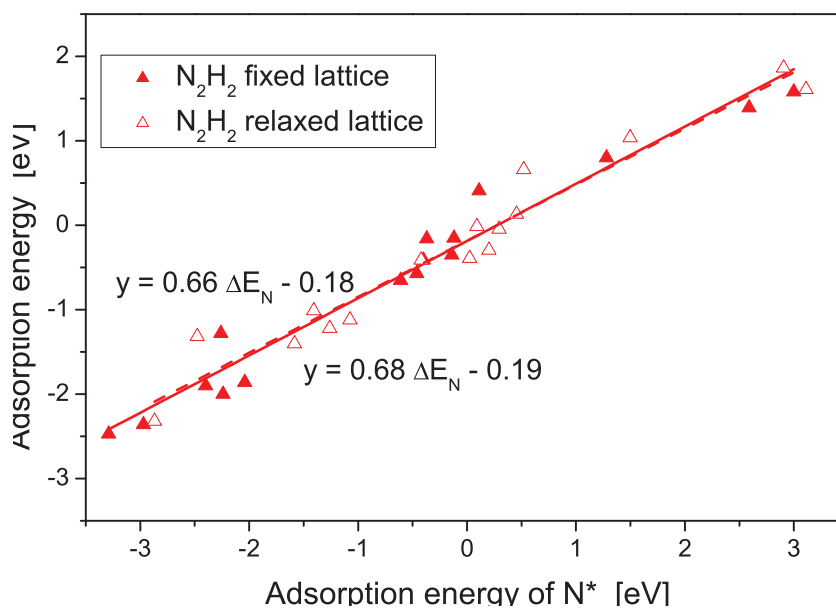


FIG. 10. The scaling relations of the N_2H_2 specie on both the bulk M12 and relaxed M12.

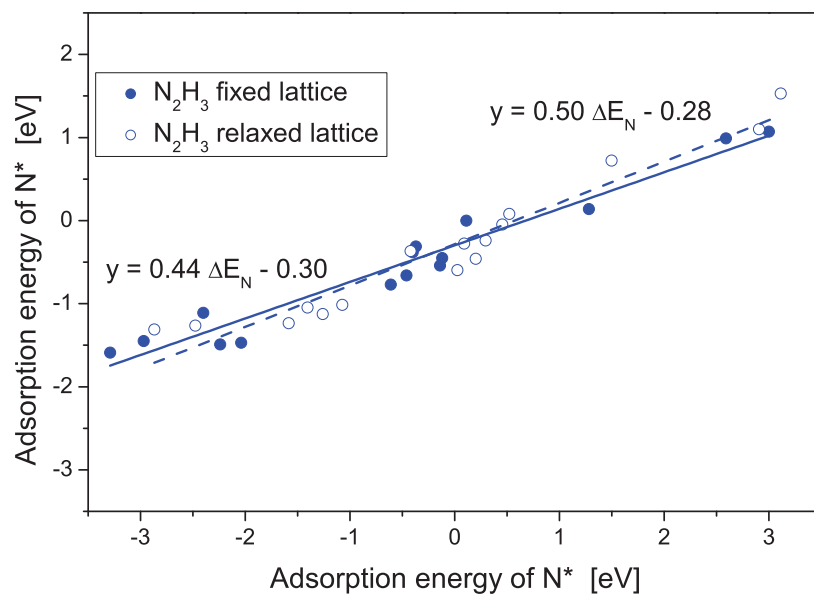


FIG. 11. The scaling relations of the N₂H₃ specie on both the bulk M12 and relaxed M12.

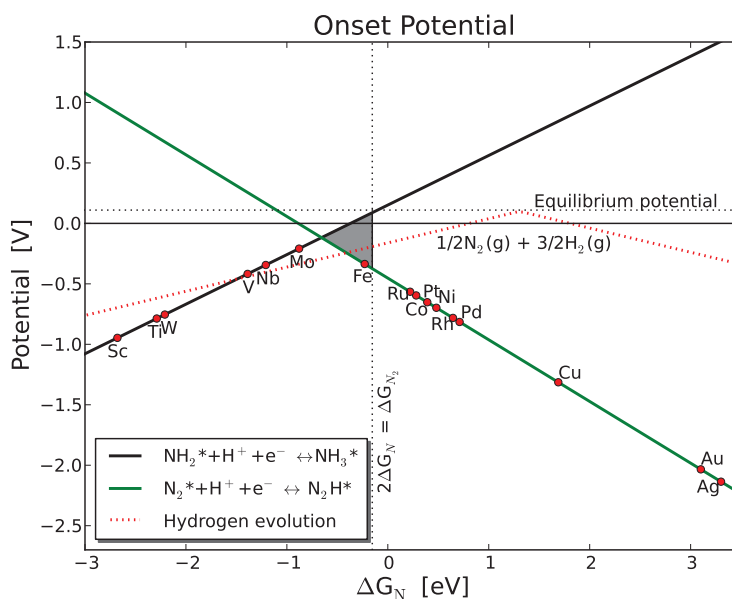


FIG. 12. The volcano plot established with no use of the calculated free energy corrections for the reaction intermediates. Leaving out the free energy corrections there is a minor shift for the top of the volcano where the free energy for adsorbed an adsorbed nitrogen adatom moves from -0.5 eV to -0.6 eV while the onset potential moves up with 0.4 eV. The potential determining step is still the same for the new volcano and the overall trend is the same, however NH_3 is now favored compared to HER. The fact that the top of the volcano is positioned close to the same free energy of adsorbed nitrogen adatom indicate that the overall trends for these very undercoordinate reaction sites are to a large degree independent on the calculated free energy corrections.