We observe from Table 4 that in terms of relaxed bond lengths, the preferred adsorption site is the one with the lowest Pd-O bond length which is where Pd_{13} is bonded to three top oxygen (3b) atoms, with a Pd-O bond length of 2.054 Å. The adsorption strength of the interaction of Pd_{13} with (110) TiO_2 was calculated using Equation 2.

Table 4. The calculated Pd-O bond length and adsorption energies of the Pd_{13}/TiO_2 (110) system.

Adsorption site	Pd-O bond length (Å)		E_{ads} (eV)
	Calc.	Exp. [19]	
O(b)	2.063	2.036	-1.746
Ti(in)	2.278	2.264	-1.438
O(in)	2.109	2.096	-2.259
O(2b)	2.083	-	-2.842
O(3b)	2.054	-	-1.815

Interestingly, compared to the bond lengths, the adsorption energies show that the preferred adsorption site is the Pd bonded to two top oxygens (2b) with an adsorption energy of -2.842 eV. This suggests that the reaction is spontaneous and exothermic.

4. Conclusion

Calculations on the lattice parameters of TiO_2 polymorphs were performed using first principles method and the results were found to be in good agreement with the available experimental data. The mechanical properties suggested that rutile is the most stable polymorph. The surface energies for the five crystallographic planes showed the (110) surface as the most stable surface with the smallest surface energy of 0.083 $eV/Å^2$. The interaction between water and the surfaces of rutile (TiO_2) was investigated, it was found that the (110) surface with water adsorbed on the oxygen site because of the most negative adsorption energy. Furthermore, the order of stability accords well with previous surface work done [17]. We have also calculated the binding energies and second difference energy of the palladium clusters and found good agreement with the experimental data [18].

The Pd_{13}/TiO_2 (110) interactions were determined by adsorbing palladium (Pd_{13}) at different adsorption sites and we observed the effect on the bond lengths and adsorption energies of the system. The adsorption energy for the Pd_{13}/TiO_2(110) suggested that the reaction is spontaneous (negative, $E_{ads}<0$). Furthermore, the Pd-Ti bond distances are comparable before and after adsorption with a slight increase from 2.057 Å to 2.278 Å. This may suggest a good catalytic reactivity of the Pd_{13}/TiO_2(110). The findings of this research may suggest that the interactions of Pd_{13}/TiO_2(110) are favorable and may be used in catalytic convertors.

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