The adsorption of furfural on $SrTiO_3$ and $SrCo_xTi_{1-x}O_3$ perovskites: A DFT study within the molecular cluster approach

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Abstract
The adsorption of furfural on $SrTiO_3$ and $SrCo_xTi_{1-x}O_3$ perovskites is addressed by DFT calculations within the molecular cluster approach. The results show that the mode of adsorption depend on the type of isomer, cis or trans. The cis isomer adsorbs through the interaction of both oxygen atoms of furfural with the surface, while the trans isomer interacts only through the carbonyl oxygen. The partial substitution of titanium by cobalt modifies importantly the adsorption modes, thus the cis isomer adsorbs by means of the simultaneous interaction of the carbonyl oxygen with the cobalt and titanium atoms, through the unshared electrons of the oxygen atom. The trans isomer instead adsorbs solely by means of the interaction of the carbonyl oxygen with the cobalt and titanium atoms.

Author keywords
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