Modifying the fullerene surface using endohedral noble gas atoms: density functional theory based molecular dynamics study of $C_{70}O_3$.

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Streszczenie

We have performed a series of ab initio molecular orbital and molecular dynamics calculations to ascertain the influence of an endohedral noble gas atom on the reactivity of the surface of the model system $C_{70}O_3$. Our simulations show that the minimum energy pathways for the ozone ring-opening reaction are influenced by the presence of the endohedral atom. The effect is isomer dependent, with the enthalpy of the reaction increasing for *a*,*b*-$C_{70}O_3$ and decreasing for *e*,*e*-$C_{70}O_3$ when doped with the heavy noble gas atoms Xe and Rn.

Adres publiczny

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https://www.acs.org/content/acs/en.html