An atom-in-molecules and electron-localization-function study of the interaction between O_2 and $V_xO_y^+/V_xO_y$ (x = 1, 2, y = 1-5) clusters.

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Rok wydania

2002

Czasopismo

Theoretical Chemistry Accounts

Numer woluminu

108

Strony

12-20

DOI

10.1007/s00214-002-0350-1

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

The most stable structures of VxOþy=VxOy(x ¼ 1, 2, y ¼ 1–5) clusters and their interaction with O_2 are determined by density functional calculations, the B3LYP functional with the 6-31G* basis set. The nature of the bonding of these clusters and the interaction with O_2 have been studied by topological analysis in the framework of both the atoms-in-molecules theory of Bader and the Becke–Edgecombe electron localization function. Bond critical points are localized by means of the analysis of the electron density gradient field, q(r), and the electron localization function gradient field, g(r). The values of the electron density properties, i.e.,

electron density, q(r), Laplacian of the electron density, 2q(r), and electron localization function, g(r), allow the nature of the bonds to be characterized, and linear correlation is found for the results obtained in both gradient fields. Vanadium-oxygen interactions are characterized as unshared-electron interactions, and linear correlation is observed between the electron density

properties and the V–O bond length. In contrast, O_2 units involve typical shared-electron interactions, as for the dioxygen molecule. Four different vanadium–oxygen interactions are found and characterized: a molecular O_2 interaction, a peroxo O_22 interaction, a superoxo O_2interaction and a side-on O_2 interaction.

Słowa kluczowe

Vanadium oxides, Clusters Bondingelectron, localization function, Topological analysis

Adres publiczny

http://dx.doi.org/10.1007/s00214-002-0350-1

Strona internetowa wydawcy

http://link.springer.com