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Strong chemisorption of E2H2 and E2H4 (E=C, Si) on B12N12 nano-cage

A. Rezaei, R. Ghiasi, A. Marjani • Published 2 May 2020 • Materials Science • Journal of Nanostructure in Chemistry

In this investigation, the adsorption behavior of E2H2 and E2H4 (E = C, Si) gas molecules on B12N12 nano-cage was studied at M062X/6-311G(d,p) level of theory. The interactions between the E2H2 and E2H4 molecules and B12N12 nano-cage were illustrated with energy decomposition analysis (EDA). Variations in the frontier orbitals energies and structural parameters were studied. Charge transfer between fragments was illustrated with electrophilicity-based charge transfer (ECT) and extended charge… Expand

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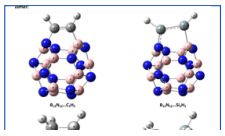
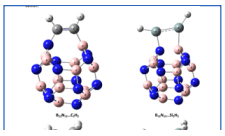


Figure 1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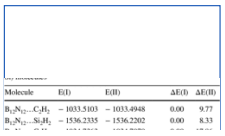
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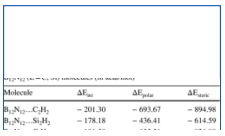
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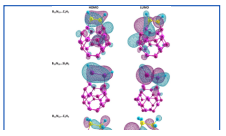
Figure 2

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Z. Rahmani, Saeed Fosshat, S. M. Alizadeh, Farzad Tat Shahdost, Mohamad Reza Poor Heravi, A. Ebadi • Monatshefte für Chemie - Chemical Monthly • 2021

The adsorption of N2, O2, H2O, hydrogen chloride (HCl), Cl2, hypochlorous acid (HClO), and ClO2 gases was explored onto an AlN nanotube (AlNNT) through density functional theory computations. As N2,… Expand

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N. Shajari, H. Yahyaei, A. Ramazani • Materials Science • 2021

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Yan Cao, S. Aslanzadeh, M. Farahmand, Sheida Ahmadi, P. D. K. Nezhad • Chemistry • 2021

Abstract The adsorption of cyanogen fluoride (FCN) was explored onto intrinsic and Ti-doped graphene-like BC3 through density functional theory computations. An energy of 3.7 to 4.6 kcal/mol is… Expand

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BF3 adsorption on pure, Al-doped, and Sc-doped graphene-like BC3: a DFT study

Jie Zhao, Wenli Li, Chunyu Song, M. Derakhshandeh • Monatshefte für Chemie - Chemical Monthly • 2021

The adsorption of boron trifluoride was explored onto pure, Al-doped, and Sc-doped BC3 nanosheets through density functional theory computations. As BF3 approaches the BC3, its adsorption releases… Expand

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Computational investigation of sensing properties of Ca-doped zinc oxide nanotube toward formaldehyde

Ji Zhou, Linhai Zou, Xiaoyi Zhang, Lixia Ji, P. D. K. Nezhad • Medicine • Journal of Molecular Modeling • 2021

TLDR Both theory and experiment suggest that Ca-doped ZnONT may be a formaldehyde gas sensor with a short recovery time. Expand

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The capability of boron carbide nanotube as a nanocarrier for fluorouracil anticancer drug delivery; DFT study

Yan Cao, S. Alamri, Ali A. Rajhi, Ali E. Anqi, M. Derakhshandeh • Materials Science • Materials Chemistry and Physics • 2022

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Pt-decorated BN nanosheets as chemical sensor for recognition of dopamine drug

Yan Cao, S. Aslanzadeh, A. SA. Alsubaie, K. H. Mahmoud, Z. Bagheri, Abdol Ghaffar Ebadi • Inorganic Chemistry Communications • 2021

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Quantum chemical studies of mercaptan gas detection with calcium oxide nanocluster

M. R. Heravi, A. Ebadi, Issa Amini, H. K. Mahmood, S. A. Alsobaei, A. Mohamadi • Medicine • Journal of Molecular Modeling • 2021

TLDR It could be concluded that Ca12O12 nanocluster has a short recovery time, as solvent considerably influences the geometry factors and electronic features of CH4S/Ca12O 12 complexes, and the interactions between species are significantly weaker in the aqueous medium compared with those in the vacuum. Expand

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References

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A DFT study on electronic and optical properties of aspirin-functionalized B12N12 fullerene-like nanocluster

E. Vessally, M. Esrafili, Roghaye Nurazar, P. Nematollahi, A. Bekhradnia • Chemistry • Structural Chemistry • 2016

In this work, the interaction of an aspirin (AS) molecule with the external surface of a boron nitride fullerene-like nanocage (B12N12) is studied by means of density functional theory (DFT)... Expand

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Adsorption of C2H2 and C2H4 on Pt-decorated graphene nanostructure: Ab-initio study

A. Rad • Chemistry • 2016

Abstract Adsorption properties of C 2 H 2 and C 2 H 4 gas molecules on Pt-decorated graphene (PtG) have been examined using first-principles density functional theory (DFT) calculations. A particular... Expand

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Why do the heavy-atom analogues of acetylene E2H2 (E = Si-Pb) exhibit unusual structures?

M. Lein, A. Krapp, G. Frenking • Chemistry, Medicine • Journal of the American Chemical Society • 2005

TLDR DFT calculations at BP86/QZ4P have been carried out with the goal to explain the unusual equilibrium geometries of the heavier group 14 homologues where E = Si-Pb, which are explained with the interactions between the EH moieties in the (X(2)Pi) electronic ground state which differ from C(2)H(2), which is bound through interactions between CH in the a(4)Sigma(-) excited state. Expand

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A Density Functional Approach toward Structural Features and Properties of C20 and its Complexes with C2X4, C2X2 (X = H, F, Cl, Br) for Synthesis Application

R. Ghiasi, Farideh Hadi, Amir Hossien Hakimyuon • Chemistry • 2014

The complexes between C20 and C2 X4 , C2 X2 (X = H, F, Cl, Br) have been studied theoretically at the B3LYP/6-311G (d,p) level. The calculations include the optimized geometries, the interaction... Expand

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Electronic and optical properties of 5-AVA-functionalized BN nanoclusters: a DFT study

A. Soltani, Ahmad Sousaraei, M. Javan, M. Eskandari, H. Balakheyli • Chemistry • 2016

We carried out detailed density functional theory (DFT) and time-dependent density functional theory (TD-DFT) calculations upon 5-aminolevulinic acid-functionalized B12N12 and B16N16 nanoclusters... Expand

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A theoretical study of the influence of solvent polarity on the structure and spectral properties in the interaction of C20 and Si2H2

R. Ghiasi, S. Jamehbozorgi, Z. Kazemi • Materials Science • 2019

In this investigation, the interaction of C20 and disilyne (Si2H2) fragment was explored in the M062X/6-311++G(d,p) level of theory in gas solution phases. The interaction energy was obtained with... Expand

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Adsorption of pyrrole on Al12N12, Al12P12, B12N12, and B12P12 fullerene-like nano-cages; a first principles study

A. Rad, K. Ayub • Chemistry • 2016

Abstract Adsorption of pyrrole on the surfaces of four X 12 Y 12 semiconductors (Al 12 N 12 , Al 12 P 12 , B 12 N 12 , and B 12 P 12) is studied through density functional theory (DFT) calculations... Expand

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Gold as hydrogen. An experimental and theoretical study of the structures and bonding in disilicon gold clusters Si2Au(n)- and Si2Au(n) (n = 2 and 4) and comparisons to Si2H2 and Si2H4.

Xi Li, B. Kiran, Lai-Sheng Wang • Chemistry, Medicine • The journal of physical chemistry. A • 2005

TLDR The H analogy of Au is more general and it is found that the chemical bonding and potential energy surfaces of two disilicon Au clusters, Si(2)Au(2) and Si (2)AU(4), are analogous to Si(2). Expand

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M. T. Nguyen, D. Sengupta, L. Vanquickenborne · Chemistry · 1995

Abstract The potential energy surface for the 1,2-hydrogen shift converting silavetylene to silylidene, HSi CH→Si=CH 2 , has been calculated by means of ab initio molecular orbital methods up to the… Expand

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Synthesis and properties of a new kinetically stabilized digermyne: new insights for a germanium analogue of an alkyne.

Y. Sugiyama, T. Sasamori, +4 authors N. Tokitoh · Chemistry, Medicine · Journal of the American Chemical Society · 2006

The reduction of an overcrowded (E)-1,2-dibromodigermene, Bbt(Br)Ge=Ge(Br)Bbt (2) [Bbt = 2,6-bis[bis(trimethylsilyl)methyl]-4-[tris(trimethylsilyl)methyl]phenyl], with KC8 afforded a stable… Expand

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