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Many-body effects on the structures and stability of Ba₂+Xe_n (n=1-39, 54) clusters

By: Abdessalem, K (Abdessalem, Kawther)^[1]; Habli, H (Habli, Hela)^[1]; Ghalla, H (Ghalla, Houcine)^[1]; Yaghmour, SJ (Yaghmour, Saud Jamil)^[2]; Calvo, F (Calvo, Florent)^[3,4]; Oujia, B (Oujia, Brahim)^[1,2]

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JOURNAL OF CHEMICAL PHYSICS

Volume: 141 Issue: 15

Article Number: 154308

DOI: 10.1063/1.4896607

Published: OCT 21 2014

[View Journal Impact](#)

Abstract

The structures and relative stabilities of mixed Ba₂+ Xe-_n (n = 1-39, 54) clusters have been theoretically studied using basin-hopping global optimization. Analytical potential energy surfaces were constructed from ab initio or experimental data, assuming either purely additive interactions or including many-body polarization effects and the mutual contribution of self-consistent induced dipoles. For both models the stable structures are characterized by the barium cation being coated by a shell of xenon atoms, as expected from simple energetic arguments. Icosahedral packing is dominantly found, the exceptional stability of the icosahedral motif at n = 12 being further manifested at the size n = 32 where the basic icosahedron is surrounded by a dodecahedral cage, and at n = 54 where the transition to multilayer Mackay icosahedra has occurred. Interactions between induced dipoles generally tend to decrease the Xe-Xe binding, leading to different solvation patterns at small sizes but also favoring polyicosahedral growth. Besides attenuating relative energetic stability, many-body effects affect the structures by expanding the clusters by a few percents and allowing them to deform more. (C) 2014 AIP Publishing LLC.

Keywords

KeyWords Plus: KXEN POLYATOMIC EXCIPLEXES; NOBLE-GAS CLUSTERS; FINITE-TEMPERATURE SPECTROSCOPY; DER-WAALS CLUSTERS; ALKALI-METAL ION; MONTE-CARLO; AB-INITIO; NA ATOMS; DYNAMICS SIMULATIONS; GLOBAL OPTIMIZATION

Author Information

Reprint Address: Abdessalem, K (reprint author)

+ Univ Monastir, Fac Sci Monastir, Lab Phys Quant, Ave Environm, Monastir 5019, Tunisia.

Addresses:

+ [1] Univ Monastir, Fac Sci Monastir, Lab Phys Quant, Monastir 5019, Tunisia

+ [2] King Abdulaziz Univ, Fac Sci, Phys Dept, Jeddah, Saudi Arabia

+ [3] Univ Grenoble Alpes, LIPHY, F-38000 Grenoble, France

+ [4] CNRS, LIPHY, F-38000 Grenoble, France

E-mail Addresses: kawtherabdessalem@yahoo.fr

Publisher

AMER INST PHYSICS, 1305 WALT WHITMAN RD, STE 300, MELVILLE, NY 11747-4501 USA

Categories / Classification

Research Areas: Chemistry; Physics

Web of Science Categories: Chemistry, Physical; Physics, Atomic, Molecular & Chemical

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