An investigation into the physical, chemical and thermochemical properties of Niobium nanoclusters.

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Abstract

The search for spin-polarized metal clusters, energetic crystals and conductive materials is a paramount part of Nanotechnology. Adapting quantum chemistry and quantum mechanics methods to study and endeavor the electronic and lattice properties of groups of atoms in nanoclusters is a central approach, which aids in revealing crucial electronic properties that serve to develop and synthesize nanomaterials, nanometals and metal clusters. This project investigates the energy landscape of Niobium clusters (Nb), in order to shed light on their electronic, dipole, and magnetic properties. The clusters are studied with the XTB Tight-binding software coupled with hybrid DFT functionals. The results show that Niobium clusters in nanosized particles (10-61 atoms) bear ultra-low orbital gaps, with promising properties for hyperconnects and nanoparticle based electronics.

Introduction

Niobium (Nb) is a superconductor element [1] and is used for a range of various metallic properties, such as aerospace engineering, space programs and also in thermoresistant applications [2]. Novel innovations include the application of Nb-composites as interface stabilizers for high-temperature applications, given its high stability towards oxidizing conditions [3], while other applications include nanoelectronic devices applied for memory and data-storage purposes composed of Nb2O5 [4].

This project, an investigation is made into the energy landscapes, physical and thermochemical properties of different Niobium crystals, encompassing several geometries in their neutral states. The size and geometries of the clusters is expected to give crucial insights into the distribution of electrons, the electronic properties and magnetic and electric characteristics. The results herein are important to develop new technologies based on the use transition metals as small particles, as also components in quantum computing devices.

Materials and Methods

Niobium crystals were build with the Amsterdam Density Functional suite [5] by constructing a bcc lattice of Niobium of dimensions 7x7x7 Å. The central atom was pinpointed, and the surrounding atoms in a radius of 6 Å were selected. This generated the source crystal, composed of 61 atoms, from which all substructures were generated. Atoms were removed in a symmetric manner, generating the configurations shown in Figure 1. All large geometries were assigned neutral charges, as only neutral species are studied in this work. This generated a total of XNiobium input configurations which were optimised geometrically using Grimme’s tight-binding XTB program v. 5.6.45 [6].

Figure 1. The converged Niobium nanocluster structures. From left to right in sequential order: Nb61, Nb53, Nb47, Nb37, Nb27, Nb21, Nb17, Nb11. Top half: Ball and stick models generated in Molden [7]. Lower half: Surface models generated in PyMol [8].

The remaining clusters, the large set (Fig 4) contains four members of Nb clusters with preserved Cmmm geometries, (ccm) except the Nb25 cluster that displays a D5h geometry. The bond lengths are respectively preserved in the interval 2.67-3.28Å for all the major clusters, and the clusters pertain the bcc geometry in their inner core. The electronic properties differ considerably, and are shown in Table 1.


Conclusions

The current results show that Niobium atoms may assemble in spherical hollow cages when the number of atoms is between 20 and 30. These nanoclusters have, although the particular symmetries are preserved, yields non-convergence in the quantum chemical calculations.

References