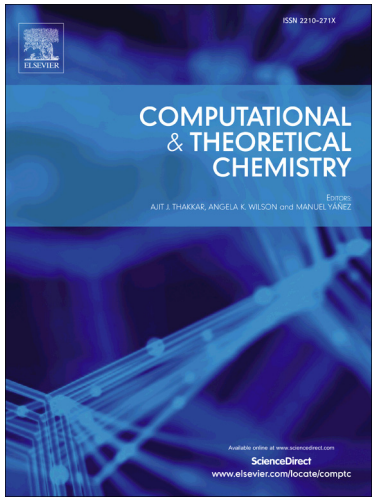
Accepted Manuscript



Combining shape-changing with exchange moves in the optimization of nano-alloys

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PII: S2210-271X(17)30002-6
DOI: http://dx.doi.org/10.1016/j.comptc.2017.01.002
Reference: COMPTC 2361

To appear in: *Computational & Theoretical Chemistry*

Received Date: 14 November 2016
Revised Date: 2 January 2017
Accepted Date: 3 January 2017

Please cite this article as: G. Rossi, R. Ferrando, Combining shape-changing with exchange moves in the optimization of nanoalloys, *Computational & Theoretical Chemistry* (2017), doi: http://dx.doi.org/10.1016/j.comptc.2017.01.002

Combining shape-changing with exchange moves in the optimization of nanoalloys

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Abstract

The search for the lowest potential energy configuration of nanoalloys is a challenging global optimization problem. As size increases above 100 atoms (~ 1.5 nm), the optimization of the structure and, at the same time, of the chemical order of the two metal components becomes extremely challenging. Here we present an implementation of the popular basin-hopping algorithm for the optimization of the potential energy of nanoclusters that combines two different types of moves, namely shape-changing moves and exchange moves. The latter, aimed at the exploration of the nanoalloy homotops via swapping of pairs of atoms of different species, can be tailored to maximize their efficiency based on the *a priori* knowledge of few physical features of the metals composing the nanoalloy. We demonstrate the performance of our approach on nanoalloys of 400 atoms composed by Au and Rh (a phase-separating binary system) or by Au and Cu (a miscible system forming ordered alloys in the bulk). Our results show that the combination of shape-changing an exchange moves can boost the optimization performance, provided that each move is associated to a different acceptance temperature in the basin hopping scheme.

Keywords: nanoalloys, optimization, copper, gold, rhodium

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