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HRMC_2.1: Hybrid Reverse Monte Carlo method with silicon, carbon, germanium and silicon carbide potentials

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ABSTRACT

The Hybrid Reverse Monte Carlo (HRMC) code models the atomic structure of materials via the use of a combination of constraints including experimental diffraction data and an empirical energy potential. In this version 2.1 update, an empirical potential for silicon-carbide has been added to the code along with an experimentally motivated constraint on the bond type fraction applicable to systems containing multiple elements.

New version program summary

Program title: HRMC version 2.1

Catalogue identifier: AEAO_v2_1

Program summary URL: http://cpc.cs.qub.ac.uk/summaries/AEAO_v2_1.html

Program obtainable from: CPC Program Library, Queen's University, Belfast, N. Ireland

Licensing provisions: Standard CPC licence, http://cpc.cs.qub.ac.uk/licence/licence.html

No. of lines in distributed program, including test data, etc.: 114 084

No. of bytes in distributed program, including test data, etc.: 1289 369

Distribution format: tar.gz

Programming language: FORTRAN 90.

Computer: any computer capable of running executables produced by the Fortran 90 compiler. For example, the code runs in Windows 7, once compiled with the GNU Fortran 95 compiler.

Operating system: Unix, Windows.

Classification: 7.7.

Catalogue identifier of previous version: AEAO_v2_0

Journal reference of previous version: Comput. Phys. Comm. 184 (2013) 1946

Does the new version supersede the previous version?: yes

Nature of problem:
atomic modelling using a combination of empirical potentials, fits to experimental data and other chemically or physically motivated constraints.

Solution method:
single move Metropolis Monte Carlo method used to minimize the total energy and discrepancy between simulation and experimental data.

Reasons for new version:
extension of capabilities from old version.

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Summary of revisions:

1. Inclusion of a bond-order potential for silicon carbide (P. Erhart, K. Albe, Phys. Rev. B 71 (2005) 035211). The selection of this potential is via the POT_TYPE parameter in the HRMC.inp file and the number of carbon and silicon atoms needs to be specified via the configA and configB parameters.
2. Inclusion of a constraint on the bond type fraction for multi-elemental systems. If a simulation has elements A, B and C, this constraint allows one to fix for element A, the fraction of A–A, A–B and A–C bonds (which should sum to unity) and similarly for elements B and C. The constraint is turned on via the BT_OPTION in the HRMC.inp file and it has its constraint weightings labelled in each stage alongside the other constraint weightings. The BT_OPT(1), BT_OPT(2) and BT_OPT(3) parameters are used to select which elements have their bond type fractions fitted via this constraint.
3. A new file is output called data_xyzdetail.dat. This file contains lists of the neighbour separations, bond angles and dihedral angles.
4. The header file hrmc.h has been replaced with hrmc_data.f90 which replaces the common block with a module to define global variables.

Running time:
1000 s for test run on a Intel Xeon 2.93 GHz—Nehalem series processor