An e-infrastructure for software, training and consultancy in simulation and modelling

Resultados

Información del proyecto

E-CAM

Identificador del acuerdo de subvención:
676531

Sitio web del proyecto

DOI
10.3030/676531

Proyecto cerrado

Fecha de la firma de la CE
28 Julio 2015

Fecha de inicio
1 Octubre 2015

Fecha de finalización
31 Marzo 2021

Financiado con arreglo a
EXCELLENT SCIENCE - Research Infrastructures

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Aportación de la UE
€ 4 836 895,75

Coordinado por
ECOLE POLYTECHNIQUE FEDERALE DE LAUSANNE
Switzerland

CORDIS proporciona enlaces a los documentos públicos y las publicaciones de los proyectos de los programas marco HORIZONTE.

Los enlaces a los documentos y las publicaciones de los proyectos del Séptimo Programa Marco, así como los enlaces a algunos tipos de resultados específicos,

como conjuntos de datos y «software», se obtienen dinámicamente de OpenAIRE.

Resultado final

Documents, reports (26)

E-CAM Public Wiki-like pages and newsletters III
Report on (a) the generation and updating of Wiki-like pages describing E-CAM's activities in a language appropriate to the general public; and, (b) E-CAM newsletters; published in previous 4 quarters.

E-CAM software Porting porting and Benchmarking benchmarking Data data IV
Update on E-CAM software porting and benchmarking data III.

ESDW guidelines and programme IV
Updated guidelines for format, content and coding styles in the ESWD, and programme for year 4. Drafted jointly by CH, JUELICH, ICHEC and NUID UCD. Includes updated advanced on-line training modules on use of a structured Wiki-like page, basic parallel programming, scripting tools, use of version control tools.

E-CAM Public Wiki-like pages and newsletters V
Report on (a) the generation and updating of Wiki-like pages describing E-CAM's activities in a language appropriate to the general public; and, (b) E-CAM newsletters; published in previous 3 quarters.

ESDW guidelines and programme III
Updated guidelines for format, content and coding styles in the ESWD, and programme for year 3. Drafted jointly by CH, JUELICH, ICHEC and NUID UCD. Includes updated on-line training modules on use of a structured Wiki-like page, basic parallel programming, scripting tools, use of version control tools..

Identification/selection of E-CAM MD codes for development
It will contain a review of software and algorithms in the area of classical MD and a list of new software to be developed at E-CAM.

E-CAM software porting and benchmarking data I
Joint technical report on results of (a) porting and optimisation of at least 8 new modules related to those developed in the ESDWs to massively parallel machine (STFC); and (b) benchmarking and scaling of at least 8 new modules related to those developed in the ESDWs on a variety of architectures (Juelich).

Identification/selection of E-CAM meso and multi-scale modelling codes for development

Special report on the state of the art methods and algorithms, including: use of neural networks for force calculation and structure recognition; kinetic Monte Carlo calculations and the interface with computational fluid dynamics and electronic structure calculations; charge and polarization in dissipative dynamics calculations; statistical mechanics of Hamiltonian adaptive resolution simulations; hybrid kinetic schemes for modeling complex fluidsIt will also contain a review of software in this area and a list of new modules to be developed by E-CAM.

E-CAM software porting and benchmarking data II

E-CAM software porting and benchmarking data I.

ESDW guidelines and programme V

Updated guidelines for format, content and coding styles in the ESWD, and programme for year 5. Drafted jointly by CH, JUELICH, ICHEC and NUID UCD. Updated advanced on-line training modules on use of a structured Wiki-like page, basic parallel programming, scripting tools, use of version control tools.

Hardware developments V

Update on hardware developments IV.

Hardware developments III

Update on hardware developments II.

E-CAM software porting and benchmarking data III

E-CAM software platform I

On-line publication of the E-CAM web-platform. The platform will include: (a) the E-CAM library of software modules and interfaces; (b) end users portal (to access E-CAM's resources, make requests for software developments, register for events); (c) web infrastructure for teaching tools.

ESDW guidelines and programme I

Guidelines for format, content and coding styles in the ESWD, and programme for year 1. Drafted jointly by CH, JUELICH, ICHEC and NUID UCD. Includes 4-8 advanced on-line training modules on use of a structured Wiki-like page, basic parallel programming, scripting tools, use of version control tools.

E-CAM software porting and benchmarking data V

Update on E-CAM software porting and benchmarking data IV.

E-CAM Public Wiki-like pages and newsletters II

E- CAM Public Wiki-like pages and newsletters II

E-CAM Public Wiki-like pages and newsletters I

Report on (a) the generation and updating of Wiki-like pages describing E-CAM's activities in a language appropriate to the general public; and, (b) E-CAM newsletters; published in previous 4 quarters.

ESDW guidelines and programme II

Updated guidelines for format, content and coding styles in the ESWD, and programme for year 2. Drafted jointly by CH, JUELICH, ICHEC and NUID UCD. Includes updated on-line training modules on use of a structured Wiki-like page, basic parallel programming, scripting tools, use of version control tools.

Hardware developments IV

Update on hardware developments III.

Identification/selection of E-CAM electronic structure codes for development

Special report on the state of the art codes and methods in Quantum Monte Carlo and Density Functional Theory (DFT) and beyond DFT methods. It will contain a review of the basic features that the majority of these codes have in common with a view to modularisation. It will also contain a review of software in this area and a list of new modules to be developed by E-CAM.

E-CAM Public Wiki-like pages and newsletters IV

Report on (a) the generation and updating of Wiki-like pages describing E-CAM's activities in a language appropriate to the general public; and, (b) E-CAM newsletters; published in previous 4 quarters.

Hardware developments I

Joint report by STFC FR-IDF, and ICHEC on: (a) Report on hardware developments that will affect the scientific areas of interest to E-CAM and detailed feedback to the project software developers (STFC); (b) discussion of project software needs with hardware and software vendors, completion of survey of what is already available for particular hardware platforms (FR-IDF); and, detailed output from direct face-to-face session between the project end-users, developers and hardware vendors (ICHEC).

Identification/selection of E-CAM quantum dynamics codes for development

Special report on the state of the art algorithms and efficient methods and interfaces for coupling electronic structure and quantum dynamical calculations. A list of new modules to be developed by E-CAM will also be provided.

Hardware developments II

Update on Hardware developments I.

ESDW technical software guidelines I

Guidelines for technical development of the software modules and the general E-CAM software architecture.

Other (25)

Electronic structure E-CAM modules III

9 software modules delivered to the E-CAM repository in the area of Electronic Structure responding to requests of users, and their documentation.

Quantum dynamics E-CAM modules III

6 software modules delivered to the E-CAM repository in the area of Quantum Dynamics based on users requests and their documentation.

Classical MD E-CAM modules V

Final Software modules delivered to the E-CAM repository in the area of Classical Molecular Dynamics responding to requests of users, and their documentation.

Meso and multi-scale modelling E-CAM modules IV

9 Software modules delivered to the E-CAM repository in the area of Meso and Multi-Scale Modelling responding to requests of users, and their documentation.

E-CAM software platform II

Update on E-CAM software tools and platforms jointly by CH and Juelich.

E-CAM software platform III

Update on E-CAM software tools and platforms jointly by CH and Juelich.

Classical MD E-CAM modules II

9 software modules delivered to the E-CAM repository in the area of statistical and machine learning tools for the analysis of rare events, and their documentation.

Electronic structure E-CAM modules V

Final software modules delivered to the E-CAM repository in the area of Electronic Structure responding to requests of users, and their documentation.

Meso and Multimulti-scale modelling E-CAM modules II

9 software modules delivered to the E-CAM repository in the area of meso and multi-scale modelling, based on user requests and their documentation.

Quantum Dynamics dynamics E-CAM modules V

Final software modules delivered to the E-CAM library in the area of Quantum Dynamics based on users requests and their documentation.

Electronic structure E-CAM modules II

9 software modules delivered to the E-CAM repository in the area of Wannier90 and electron phonon Wannier calculations.

Classical MD E-CAM modules III

9 software modules delivered to the E-CAM repository in the area of classical molecular dynamics responding to requests of users, and their documentation.

Meso and multi-scale modelling E-CAM modules V

Final Software modules delivered to the E-CAM repository in the area of meso and mulit-scale modelling responding to requests of users, and their documentation.

Classical MD E-CAM modules IV

9 software modules delivered to the E-CAM repository in the area of Classical Molecular Dynamics responding to requests of users, and their documentation.

E-CAM software platform IV

Update on E-CAM software tools and platforms jointly by CH and Juelich.

E-CAM software platform V

Update on E-CAM software tools and platforms jointly by CH and Juelich.

Meso and multi-scale modelling E-CAM modules I

9 software modules delivered to the E-CAM repository in the area of meso and multi-scale modelling, and their documentation.

Classical MD E-CAM modules I

9 software modules in classical Molecular Dynamics delivered to the E-CAM repository in the area of trajectory sampling, thermodynamics and kinetics of rare events, and their documentation.

Meso and multi-scale modelling E-CAM modules III

9 software modules delivered to the E-CAM repository in the area of meso and multi-scale modelling, based on user requests and their documentation.

Quantum dynamics E-CAM modules IV

6 software modules delivered to the ECAM repository in the area of Quantum Dynamics based on users requests and their documentation

Electronic structure E-CAM modules I

9 Software modules delivered to the E-CAM library in electronic structure including solvers for localised orbitals, for computing on a grid and solvers, and for transport, and their documentation.

Quantum dynamics E-CAM modules II

6 software modules delivered to the E-CAM repository in the area of quantum dynamics based on user requests and their documentation.

Electronic structure E-CAM modules IV

9 Software modules delivered to the E-CAM repository in the area of Electronic Structure responding to requests of users, and their documentation.

Quantum dynamics ECAM modules I

6 software modules delivered to the E-CAM repository in the areas of: (1) approximate methods for computing quantum time correlation functions; (2) exact integrators for the Schroedinger equation; (3) model potentials of increasing complexity for benchmarking

E-CAM software development tools

On-line deployment of centralized tools for software development, documentation and maintenance. These will include tools for automatic extraction of software documentation, bug tracking, version control, low-level software (e.g. memory handling).

Open Research Data Pilot (1)

Data Management Plan

The Project Administrator will develop a Data Management Plan (DMP) with all the participants. It will describe in detail how reports and data are handled. The plan will be approved and owned by the Executive Management Team. The plan, that outlines the practices for collecting, organizing, backing-up, and storing the data, will be updated regularly throughout the project. Within this task the data management plan for the Pilot on Open Research Data will be defined and delivered. It will outline how the data, including associated metadata, needed to validate the results presented in scientific publications will be made available openly.

Publicaciones

Peer reviewed articles (42)

Atomistic insight into the kinetic pathways for Watson–Crick to Hoogsteen transitions in DNA
Autores: Jocelyne Vreede, Alberto Pérez de Alba Ortíz, Peter G Bolhuis, David W H Swenson
Publicado en: Nucleic Acids Research, Edición 47/21, 2019, Página(s) 11069-11076, ISSN 0305-1048
Editor: Oxford University Press
DOI: 10.1093/nar/gkz837

Electronic structure and optical properties of quantum crystals from first principles calculations in the Born–Oppenheimer approximation
Autores: Vitaly Gorelov, David M. Ceperley, Markus Holzmann, Carlo Pierleoni
Publicado en: The Journal of Chemical Physics, Edición 153/23, 2020, Página(s) 234117, ISSN 0021-9606
Editor: American Institute of Physics
DOI: 10.1063/5.0031843

Unfolding the prospects of computational (bio)materials modeling
Autores: G. J. Agur Sevink, Jozef Adam Liwo, Pietro Asinari, Donal MacKernan, Giuseppe Milano, Ignacio Pagonabarraga
Publicado en: The Journal of Chemical Physics, Edición 153/10, 2020, Página(s) 100901, ISSN 0021-9606
Editor: American Institute of Physics
DOI: 10.1063/5.0019773

Microswimmers learning chemotaxis with genetic algorithms
Autores: Hartl, Benedikt; Hübl, Maximilian; Kahl, Gerhard; Zöttl, Andreas
Publicado en: PNAS, Edición 55, 2021, Página(s) in press, ISSN 1091-6490
Editor: National academy of sciences
DOI: 10.1073/pnas.2019683118

PANNA: Properties from Artificial Neural Network Architectures
Autores: Ruggero Lot, Franco Pellegrini, Yusuf Shaidu, Emine Küçükbenli
Publicado en: Computer Physics Communications, Edición 256, 2020, Página(s) 107402, ISSN 0010-4655
Editor: Elsevier BV
DOI: 10.1016/j.cpc.2020.107402

Towards blood flow in the virtual human: efficient self-coupling of HemeLB
Autores: J. W. S. McCullough, R. A. Richardson, A. Patronis, R. Halver, R. Marshall, M. Ruefenacht, B. J. N. Wylie, T. Odaker, M. Wiedemann, B. Lloyd, E. Neufeld, G. Sutmann, A. Skjellum, D. Kranzlmüller, P. V. Coveney

Publicado en: Interface Focus, Edición 11/1, 2021, Página(s) 20190119, ISSN 2042-8898
Editor: Royal Society Publishing
DOI: 10.1098/rsfs.2019.0119

Reliable Computational Prediction of the Supramolecular Ordering of Complex Molecules under Electrochemical Conditions
Autores: Benedikt Hartl, Shubham Sharma, Oliver Brügner, Stijn F. L. Mertens, Michael Walter, Gerhard Kahl
Publicado en: Journal of Chemical Theory and Computation, Edición 16/8, 2020, Página(s) 5227-5243, ISSN 1549-9618
Editor: American Chemical Society
DOI: 10.1021/acs.jctc.9b01251

Equilibrium structures of anisometric, quadrupolar particles confined to a monolayer
Autores: Thomas Heinemann, Moritz Antlanger, Martial Mazars, Sabine H. L. Klapp, Gerhard Kahl
Publicado en: The Journal of Chemical Physics, Edición 144/7, 2016, Página(s) 074504, ISSN 0021-9606
Editor: American Institute of Physics
DOI: 10.1063/1.4941585

Gap variability upon packing in organic photovoltaics
Autores: D. López-Durán, Etienne Plésiat, Michal Krompiec, Emilio Artacho
Publicado en: PLOS ONE, Edición 15/6, 2020, Página(s) e0234115, ISSN 1932-6203
Editor: Public Library of Science
DOI: 10.1371/journal.pone.0234115

Sampling the thermal Wigner density via a generalized Langevin dynamics
Autores: Thomas Plé, Simon Huppert, Fabio Finocchi, Philippe Depondt, Sara Bonella
Publicado en: The Journal of Chemical Physics, Edición 151/11, 2019, Página(s) 114114, ISSN 0021-9606
Editor: American Institute of Physics
DOI: 10.1063/1.5099246

Improved Description of Atomic Environments using Low-cost Polynomial Functions with Compact Support
Autores: Martin Peter Bircher, Andreas Singraber, Christoph Dellago
Publicado en: Machine Learning: Science and Technology, 2021, ISSN 2632-2153
Editor: IOP Publishing Ltd
DOI: 10.1088/2632-2153/abf817

Towards extreme scale dissipative particle dynamics simulations using multiple GPGPUs
Autores: Jony Castagna, Xiaohu Guo, Michael Seaton, Alan O'Cais
Publicado en: Computer Physics Communications, Edición 251, 2020, Página(s) 107159, ISSN 0010-4655
Editor: Elsevier BV
DOI: 10.1016/j.cpc.2020.107159

The Fluctuation–Dissipation Theorem as a Diagnosis and Cure for Zero-Point Energy Leakage in Quantum Thermal Bath Simulations
Autores: Etienne Mangaud, Simon Huppert, Thomas Plé, Philippe Depondt, Sara Bonella, Fabio Finocchi
Publicado en: Journal of Chemical Theory and Computation, Edición 15/5, 2019, Página(s) 2863-2880, ISSN 1549-9618
Editor: American Chemical Society
DOI: 10.1021/acs.jctc.8b01164

Adiabatic motion and statistical mechanics via mass-zero constrained dynamics
Autores: Sara Bonella, Alessandro Coretti, Rodolphe Vuilleumier, Giovanni Ciccotti
Publicado en: Physical Chemistry Chemical Physics, Edición 22/19, 2020, Página(s) 10775-10785, ISSN 1463-9076
Editor: Royal Society of Chemistry
DOI: 10.1039/d0cp00163e

A molecular perspective on Tully models for nonadiabatic dynamics
Autores: Lea M. Ibele, Basile F. E. Curchod
Publicado en: Physical Chemistry Chemical Physics, Edición 22/27, 2020, Página(s) 15183-15196, ISSN 1463-9076
Editor: Royal Society of Chemistry
DOI: 10.1039/d0cp01353f

A systematic approach to generating accurate neural network potentials: the case of carbon
Autores: Yusuf Shaidu, Emine Küçükbenli, Ruggero Lot, Franco Pellegrini, Efthimios Kaxiras, Stefano de Gironcoli
Publicado en: npj Computational Materials, Edición 7/1, 2021, ISSN 2057-3960
Editor: Nature publishing group
DOI: 10.1038/s41524-021-00508-6

Rich Polymorphic Behavior of Wigner Bilayers
Autores: Moritz Antlanger, Gerhard Kahl, Martial Mazars, Ladislav Šamaj, Emmanuel Trizac
Publicado en: Physical Review Letters, Edición 117/11, 2016, ISSN 0031-9007
Editor: American Physical Society
DOI: 10.1103/physrevlett.117.118002

Probing spatial locality in ionic liquids with the grand canonical adaptive resolution molecular dynamics technique

Autores: B. Shadrack Jabes, C. Krekeler, R. Klein, L. Delle Site
Publicado en: The Journal of Chemical Physics, Edición 148/19, 2018, Página(s) 193804, ISSN 0021-9606
Editor: American Institute of Physics
DOI: 10.1063/1.5009066

The opposing effects of isotropic and anisotropic attraction on association kinetics of proteins and colloids

Autores: Arthur C. Newton, Ramses Kools, David W. H. Swenson, Peter G. Bolhuis
Publicado en: The Journal of Chemical Physics, Edición 147/15, 2017, Página(s) 155101, ISSN 0021-9606
Editor: American Institute of Physics
DOI: 10.1063/1.5006485

Force Field Parametrization of Metal Ions from Statistical Learning Techniques

Autores: Francesco Fracchia, Gianluca Del Frate, Giordano Mancini, Walter Rocchia, Vincenzo Barone
Publicado en: Journal of Chemical Theory and Computation, Edición 14/1, 2017, Página(s) 255-273, ISSN 1549-9618
Editor: American Chemical Society
DOI: 10.1021/acs.jctc.7b00779

ζ-Glycine: insight into the mechanism of a polymorphic phase transition

Autores: Craig L. Bull, Giles Flowitt-Hill, Stefano de Gironcoli, Emine Küçükbenli, Simon Parsons, Cong Huy Pham, Helen Y. Playford, Matthew G. Tucker
Publicado en: IUCrJ, Edición 4/5, 2017, Página(s) 569-574, ISSN 2052-2525
Editor: International Union of Crystallography (IUCr)
DOI: 10.1107/S205225251701096X

Benchmarking a Fast Proton Titration Scheme in Implicit Solvent for Biomolecular Simulations

Autores: Fernando Luís Barroso da Silva, Donal MacKernan
Publicado en: Journal of Chemical Theory and Computation, Edición 13/6, 2017, Página(s) 2915-2929, ISSN 1549-9618
Editor: American Chemical Society
DOI: 10.1021/acs.jctc.6b01114

Ionic Liquids Treated within the Grand Canonical Adaptive Resolution Molecular Dynamics Technique

Autores: B. Shadrack Jabes and Christian Krekeler
Publicado en: Computation, Edición 6/1, 2018, Página(s) 23, ISSN 2079-3197

Editor: MDPI
DOI: 10.3390/computation6010023

A parallel orbital-updating based plane-wave basis method for electronic structure calculations
Autores: Yan Pan, Xiaoying Dai, Stefano de Gironcoli, Xin-Gao Gong, Gian-Marco Rignanese, Aihui Zhou
Publicado en: Journal of Computational Physics, Edición 348, 2017, Página(s) 482-492, ISSN 0021-9991
Editor: Academic Press
DOI: 10.1016/j.jcp.2017.07.033

Towards open boundary molecular dynamics simulation of ionic liquids
Autores: Christian Krekeler, Luigi Delle Site
Publicado en: Phys. Chem. Chem. Phys., Edición 19/6, 2017, Página(s) 4701-4709, ISSN 1463-9076
Editor: Royal Society of Chemistry
DOI: 10.1039/C6CP07489H

Computational efficiency and Amdahl's law for the adaptive resolution simulation technique
Autores: Christoph Junghans; Animesh Agarwal; Luigi Delle Site
Publicado en: Computer Physics Communications, Edición 1, 2017, ISSN 0010-4655
Editor: Elsevier BV
DOI: 10.1016/j.cpc.2017.01.030

ESPResSo++ 2.0: Advanced methods for multiscale molecular simulation
Autores: Horacio V. Guzman, Nikita Tretyakov, Hideki Kobayashi, Aoife C. Fogarty, Karsten Kreis, Jakub Krajniak, Christoph Junghans, Kurt Kremer, Torsten Stuehn
Publicado en: Computer Physics Communications, Edición 238, 2019, Página(s) 66-76, ISSN 0010-4655
Editor: Elsevier BV
DOI: 10.1016/j.cpc.2018.12.017

Molecular Dynamics of Open Systems: Construction of a Mean-Field Particle Reservoir
Autores: Luigi Delle Site, Christian Krekeler, John Whittaker, Animesh Agarwal, Rupert Klein, Felix Höfling
Publicado en: Advanced Theory and Simulations, Edición 2/5, 2019, Página(s) 1900014, ISSN 2513-0390
Editor: WILEY-VCH Verlag GmbH & Co.
DOI: 10.1002/adts.201900014

Unimolecular FRET sensors: Simple linker designs and properties

Autores: Shourjya Sanyal, David F. Coker, Donal MacKernan
Publicado en: Nano Communication Networks, Edición 18, 2018, Página(s) 44-50, ISSN 1878-7789
Editor: Elsevier BV
DOI: 10.1016/j.nancom.2018.10.003

Adaptive resolution molecular dynamics technique: Down to the essential
Autores: Christian Krekeler, Animesh Agarwal, Christoph Junghans, Matej Praprotnik, Luigi Delle Site
Publicado en: The Journal of Chemical Physics, Edición 149/2, 2018, Página(s) 024104, ISSN 0021-9606
Editor: American Institute of Physics
DOI: 10.1063/1.5031206

Local control theory for superconducting qubits
Autores: M. Mališ, P. Kl. Barkoutsos, M. Ganzhorn, S. Filipp, D. J. Egger, S. Bonella, I. Tavernelli
Publicado en: Physical Review A, Edición 99/5, 2019, ISSN 2469-9926
Editor: American Physical Society
DOI: 10.1103/PhysRevA.99.052316

The asymmetric Wigner bilayer
Autores: Moritz Antlanger, Gerhard Kahl, Martial Mazars, Ladislav Šamaj, Emmanuel Trizac
Publicado en: The Journal of Chemical Physics, Edición 149/24, 2018, Página(s) 244904, ISSN 0021-9606
Editor: American Institute of Physics
DOI: 10.1063/1.5053651

OpenPathSampling: A Python Framework for Path Sampling Simulations. 2. Building and Customizing Path Ensembles and Sample Schemes
Autores: David W. H. Swenson, Jan-Hendrik Prinz, Frank Noe, John D. Chodera, Peter G. Bolhuis
Publicado en: Journal of Chemical Theory and Computation, Edición 15/2, 2018, Página(s) 837-856, ISSN 1549-9618
Editor: American Chemical Society
DOI: 10.1021/acs.jctc.8b00627

Lithium Adsorption on Graphene at Finite Temperature
Autores: Yusuf Shaidu, Emine Küçükbenli, Stefano de Gironcoli
Publicado en: The Journal of Physical Chemistry C, Edición 122/36, 2018, Página(s) 20800-20808, ISSN 1932-7447
Editor: American Chemical Society
DOI: 10.1021/acs.jpcc.8b05689

Advanced capabilities for materials modelling with Quantum ESPRESSO

Autores: P Giannozzi, O Andreussi, T Brumme, O Bunau, M Buongiorno Nardelli, M Calandra, R Car, C Cavazzoni, D Ceresoli, M Cococcioni, N Colonna, I Carnimeo, A Dal Corso, S de Gironcoli, P Delugas, R A DiStasio, A Ferretti, A Floris, G Fratesi, G Fugallo, R Gebauer, U Gerstmann, F Giustino, T Gorni, J Jia, M Kawamura, H-Y Ko, A Kokalj, E Küçükbenli, M Lazzeri, M Marsili, N Marzari, F Mauri, N L Nguyen,
Publicado en: Journal of Physics: Condensed Matter, Edición 29/46, 2017, Página(s) 465901, ISSN 0953-8984
Editor: Institute of Physics Publishing
DOI: 10.1088/1361-648X/aa8f79

OpenPathSampling: A Python Framework for Path Sampling Simulations. 1. Basics

Autores: David W. H. Swenson, Jan-Hendrik Prinz, Frank Noe, John D. Chodera, Peter G. Bolhuis
Publicado en: Journal of Chemical Theory and Computation, Edición 15/2, 2018, Página(s) 813-836, ISSN 1549-9618
Editor: American Chemical Society
DOI: 10.1021/acs.jctc.8b00626

Discovering the Elusive Global Minimum in a Ternary Chiral Cluster: Rotational Spectra of Propylene Oxide Trimer

Autores: Fan Xie, Marco Fusè, Arsh S. Hazrah, Wolfgang Jäger, Vincenzo Barone, Yunjie Xu
Publicado en: Angewandte Chemie International Edition, Edición 59/50, 2020, Página(s) 22427-22430, ISSN 1433-7851
Editor: John Wiley & Sons Ltd.
DOI: 10.1002/anie.202010055

Quantum Monte Carlo determination of the principal Hugoniot of deuterium

Autores: Michele Ruggeri, Markus Holzmann, David M. Ceperley, Carlo Pierleoni
Publicado en: Physical Review B, Edición 102/14, 2020, ISSN 1098-0121
Editor: American Physical Society
DOI: 10.1103/physrevb.102.144108

Wannier90 as a community code: new features and applications

Autores: Giovanni Pizzi, Valerio Vitale, Ryotaro Arita, Stefan Blügel, Frank Freimuth, Guillaume Géranton, Marco Gibertini, Dominik Gresch, Charles Johnson, Takashi Koretsune, Julen Ibañez-Azpiroz, Hyungjun Lee, Jae-Mo Lihm, Daniel Marchand, Antimo Marrazzo, Yuriy Mokrousov, Jamal I Mustafa, Yoshiro Nohara, Yusuke Nomura, Lorenzo Paulatto, Samuel Poncé, Thomas Ponweiser, Junfeng Qiao, Florian Thöle, S
Publicado en: Journal of Physics: Condensed Matter, Edición 32/16, 2020,

Página(s) 165902, ISSN 0953-8984
Editor: Institute of Physics Publishing
DOI: 10.1088/1361-648x/ab51ff

The CECAM electronic structure library and the modular software development paradigm
Autores: Micael J. T. Oliveira, Nick Papior, Yann Pouillon, Volker Blum, Emilio Artacho, Damien Caliste, Fabiano Corsetti, Stefano de Gironcoli, Alin M. Elena, Alberto García, Víctor M. García-Suárez, Luigi Genovese, William P. Huhn, Georg Huhs, Sebastian Kokott, Emine Küçükbenli, Ask H. Larsen, Alfio Lazzaro, Irina V. Lebedeva, Yingzhou Li, David López-Durán, Pablo López-Tarifa, Martin Lüders,
Publicado en: The Journal of Chemical Physics, Edición 153/2, 2020, Página(s) 024117, ISSN 0021-9606
Editor: American Institute of Physics
DOI: 10.1063/5.0012901

Comparing equilibration schemes of high-molecular-weight polymer melts with topological indicators
Autores: Luca Tubiana, Hideki Kobayashi, Raffaello Potestio, Burkhard Dünweg, Kurt Kremer, Peter Virnau, Kostas Daoulas
Publicado en: Journal of Physics: Condensed Matter, Edición 33/20, 2021, Página(s) 204003, ISSN 0953-8984
Editor: Institute of Physics Publishing
DOI: 10.1088/1361-648x/abf20c

Automated high-throughput Wannierisation
Autores: Valerio Vitale, Giovanni Pizzi, Antimo Marrazzo, Jonathan R. Yates, Nicola Marzari, Arash A. Mostofi
Publicado en: npj Computational Materials, Edición 6/1, 2020, ISSN 2057-3960
Editor: Nature Publishing Group
DOI: 10.1038/s41524-020-0312-y

Other (1)

Intelligent HTC for Committor Analysis
Autores: O'Cais, Alan; Bialczak, Milosz; Swenson, David; Uchronsk, Mariusz; Wlodarczyk, Adam
Publicado en: PRACE White Paper, Edición 53, 2021
Editor: Zenodo
DOI: 10.5281/zenodo.4572788

Derechos de propiedad intelectual

Patent (1)

MOLECULAR SENSORS
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Conjuntos de datos

Conjuntos de datos vía OpenAIRE (3)

PANNA: Properties from Artificial Neural Network Architectures
Autores: Lot, Ruggero
Publicado en: Mendeley

Carbon configurations dataset generated in "A systematic approach to generating accurate neural network potentials: the case of carbon"
Autores: Shaidu, Yusuf; Kucukbenli, Emine; Lot, Ruggero; Pellegrini, Franco; Kaxiras, Efthimios; de Gironcoli, Stefano
Publicado en: Zenodo

Supplementary material from "Towards blood flow in the virtual human: efficient self-coupling of HemeLB"
Autores: McCullough, J. W. S.; Richardson, R. A.; A. Patronis; R. Halver; R. Marshall; M. Ruefenacht; B. J. N. Wylie; T. Odaker; M. Wiedemann; B. Lloyd; E. Neufeld; G. Sutmann; A. Skjellum; D. Kranzlmüller; Coveney, P. V.
Publicado en: The Royal Society

Otros productos de investigación

Otros productos de investigación a través de OpenAire (1)

E-CAM Case Study - Mesoscale models for polarisable solvents: application to oil-water interfaces
Autores: Silvia Chiacchiera
Publicado en: Zenodo

Última actualización: 11 Septiembre 2023

Permalink: https://cordis.europa.eu/project/id/676531/results/es