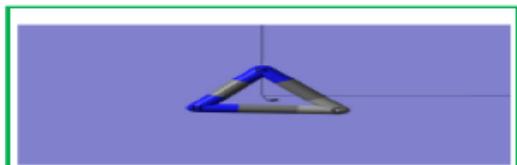
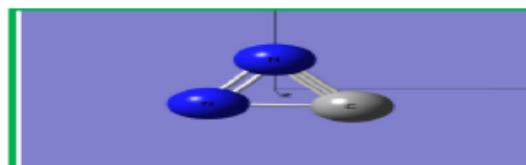




New Chemistry News



New News of Chem (NNC)



ChemNewsNew (CNN)

PetaScale Computing

Petascale Simulations of the Morphology and the Molecular Interface of Bulk Heterojunctions	ACS Nano, 2016, 10 (7), pp 7008–7022
Jan-Michael Y. Carrillo, Zach Seibers, Rajeev Kumar, Michael A. Matheson, John F. Ankner, Monojoy Goswami, Kiran Bhaskaran-Nair, William A. Shelton, Bobby G. Sumpter, and S. Michael KilbeyII	
Petascale Orbital-Free Density Functional Theory Enabled by Small-Box Algorithms	J. Chem. Theory Comput., 2016, 12 (6), pp 2950–2963
Mohan Chen, Xiang-Wei Jiang, Houlong Zhuang, Lin-Wang Wang, and Emily A. Carter	
ACS MEETING NEWS: Chemists gear up for a new generation of supercomputers	Chem. Eng. News, 2009, 87 (15), p 52
ELIZABETH WILSON	
Optimization of the Coupled Cluster Implementation in NWChem on Petascale Parallel Architectures	J. Chem. Theory Comput., 2014, 10 (10), pp 4307–4316
Victor M. Anisimov, Gregory H. Bauer, Kalyana Chadalavada, Ryan M. Olson, Joseph W. Glenski, William T. C. Kramer, Edoardo Aprà, and Karol Kowalski	
Scaling of Multimillion-Atom Biological Molecular Dynamics Simulation on a Petascale Supercomputer	J. Chem. Theory Comput., 2009, 5 (10), pp 2798–2808
Roland Schulz, Benjamin Lindner, Loukas Petridis and Jeremy C. Smith	
Calculation of Free Energy Landscape in Multi-Dimensions with Hamiltonian-Exchange Umbrella Sampling on Petascale Supercomputer	J. Chem. Theory Comput., 2012, 8 (11), pp 4672–4680
Wei Jiang, Yun Luo, Luca Maragliano, and Benoît Roux	
Placing Rigorous Bounds on Numerical Errors in Hartree–Fock Energy Computations	J. Chem. Theory Comput., 2011, 7 (6), pp 1631–1639
Pete P. Janes and Alistair P. Rendell	

Accurate Ensemble Molecular Dynamics Binding Free Energy Ranking of Multidrug-Resistant HIV-1 Proteases	J. Chem. Inf. Model., 2010, 50 (5), pp 890–905
S. Kashif Sadiq, David W. Wright, Owain A. Kenway and Peter V. Coveney	
Extrapolating Single Organic Ion Solvation Thermochemistry from Simulated Water Nanodroplets	J. Phys. Chem. B, 2016, 120 (35), pp 9402–9409
Jonathan P. Coles, Céline Houriez, Michael Meot-Ner (Mautner), and Michel Masella	

Sparse matrix factorization in the implicit finite element method on petascale architecture	Computer Methods in Applied Mechanics and Engineering 302,2016,281-292
Seid Koric and Anshul Gupta	
A high order finite difference solver for massively parallel simulations of stably stratified turbulent channel flows	Computers & Fluids 127,2016,161-173
Ping He	
A prospect for computing in porous materials research: Very large fluid flow simulations	J Computational Science 122016,62-76
Keijo Mattila and Tuomas Puurtinen and Jari Hyväluoma and Rodrigo Surmas and Markko Myllys and Tuomas Turpeinen and Fredrik Robertsén and Jan Westerholm and Jussi Timonen	
Comparing Coarray Fortran (CAF) with MPI for several structured mesh PDE applications	J Computational Physics 297,2015,237-253
Sudip Garain and Dinshaw S. Balsara and John Reid	
Deployment and testing of the sustained petascale Blue Waters system	J Computational Science 10,2015,327-337
Celso L. Mendes and Brett Bode and Gregory H. Bauer and Jeremy Enos and Cristina Beldica and William T. Kramer	
Application-specific I/O Optimizations on Petascale Supercomputers	Procedia Computer Science 29,2014,910-923
Efecan Poyraz and Heming Xu and Yifeng Cui	
Deploying a Large Petascale System: The Blue Waters Experience	Procedia Computer Science 29,2014,198-209
Celso L. Mendes and Brett Bode and Gregory H. Bauer and Jeremy Enos and Cristina Beldica and William T. Kramer,	
Performance analysis of large scale parallel CFD computing based on Code_Saturne	Computer Physics Communications 184,2013,381-386
Zhi Shang	
Adjusting process count on demand for petascale global optimization ,	Parallel Computing 39(1),2013,21-35
Masha Sosonkina and Layne T. Watson and Nicholas R. Radcliffe and Rafael T. Haftka and Michael W. Trosset	
Undergraduate Module on Computational Modeling: Introducing Modeling the Cane Toad Invasion	Procedia Computer Science 18,2013,1429-1435
Angela B. Shiflet and George W. Shiflet and Whitney E. Sanders Jr.,	
Optimizing Code_Saturne computations on Petascale systems ,	Computers & Fluids 45(1),2011,103-108
Y. Fournier and J. Bonelle and C. Moulinec and Z. Shang and A.G. Sunderland and J.C. Uribe	

Parallel application benchmarks and performance evaluation of the Intel Xeon 7500 family processors ,	Procedia Computer Science 4,2011,372-381
Piotr Kopta and Michal Kulczewski and Krzysztof Kurowski and Tomasz Piontek and Pawel Gepner and Mariusz Puchalski and Jacek Komasa,	
Unstable periodic orbits in weak turbulence	J Computational Science 1(1)2010,13-23
L. Fazendeiro and B.M. Boghosian and P.V. Coveney and J. Lätt,	
Numerical strategies towards peta-scale simulations of nanoelectronics devices	Parallel Computing 36,2010,2-3
Mathieu Luisier and Gerhard Klimeck	
A massively parallel solver for discrete Poisson-like problems ,	J Computational Physics 281,2015,237-250
Yvan Notay and Artem Napov,	
Petascale large eddy simulation of jet engine noise based on the truncated SPIKE algorithm	Parallel Computing 40(9),2014,496-511
Yingchong Situ and Chandra S. Martha and Matthew E. Louis and Zhiyuan Li and Ahmed H. Sameh and Gregory A. Blaisdell and Anastasios S. Lyrantzis,	
Asynchronous Two-level Checkpointing Scheme for Large-scale Adjoints in the Spectral-Element Solver Nek5000	Procedia Computer Science 80,2016,1147-1158
Michel Schanen and Oana Marin and Hong Zhang and Mihai Anitescu,	
I/O-aware bandwidth allocation for petascale computing systems	Parallel Computing 58,2016,107-116
Zhou Zhou and Xu Yang and Dongfang Zhao and Paul Rich and Wei Tang and Jia Wang and Zhiling Lan	
Extreme scale computing: Modeling the impact of system noise in multi-core clustered systems ,	J Parallel and Distributed Computing 73,2013,898-910
Seetharami Seelam and Liana Fong and Asser Tantawi and John Lewars , John Divirgilio and Kevin Gildea,	
Quantitative modeling of power performance tradeoffs on extreme scale systems	J Parallel and Distributed Computing 84,2015,1-14
Li Yu and Zhou Zhou and Sean Wallace and Michael E. Papka and Zhiling Lan,	
Performance Analysis and Optimization of PalaBos on Petascale Sunway BlueLight MPP Supercomputer ,	Procedia Engineering 61,2013,241-245
Tian Min and Gu Weidong and Pan Jingshan and Guo Meng,	

Credit: Acs.org