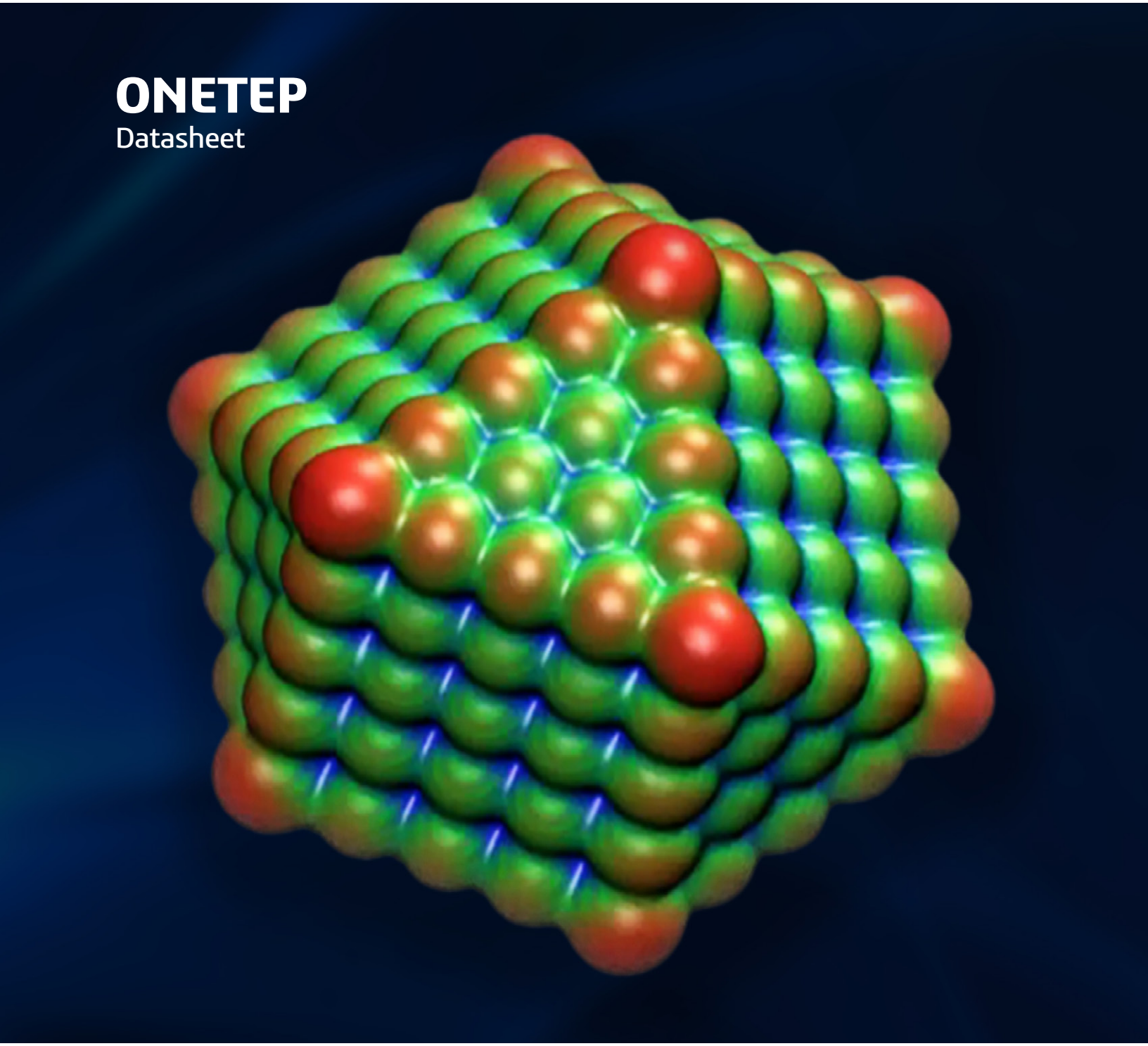
BIOVIA

3DEXPERIENCE®

ONETEP

Datasheet



DASSAULT SYSTEMES

OVERVIEW

Researchers in chemistry, pharmaceuticals, and materials science may be faced with a number of challenging goals, such as the development of new compounds or the discovery of improved manufacturing processes. As researchers treat more sophisticated problems, such as those in the realm of nanotechnology, they need to employ larger molecular models and perform calculations that provide the accuracy and reliability of quantum mechanical approaches.

In the past, this has presented a conundrum because large models were too computationally expensive to study with first-principles methods. As a result, the limitations of hardware and software forced researchers to make a give-and take decision—either use an unrealistically small model in order to obtain quantum mechanical results, or keep a realistic model but perform only an approximate calculation.

Today, it is no longer necessary to make such compromises because ONETEP delivers quantum mechanical accuracy for large systems. ONETEP is a linear scaling method, meaning the time required for a calculation increases linearly with the number of atoms. As a result of this unique scaling, the program can be used to model systems larger than possible in the past.

Typical applications of first-principles quantum mechanics calculations with ONETEP include studies of:

- surface chemistry
- structural properties of large molecular systems
- energies of protein-ligand complexes
- electronic excitations - UV/VIS spectra
- structure and energetics of nanotubes
- properties of defects (e.g. vacancies, interstitials, substitution impurities, grain boundaries, and dislocations) in semiconductors and ceramic materials

THE ONETEP ADVANTAGE — LINEAR SCALING

As illustrated by the example shown in Figure 1, the main advantage of ONETEP is its linear-scaling behavior, which means that the time required for calculating the total energy increases linearly with the number of atoms. This linear-scaling approach is a vast improvement over conventional DFT methods, where the time needed for computation typically increases at a rate of N^3 (where N is the total number of atoms).

ONETEP also runs very efficiently on multiprocessor computers, scaling to thousands of processors. Consequently, with the ONETEP module in BIOVIA Materials Studio, it is feasible to perform DFT calculations on very large systems (even ones with thousands of atoms). It is also possible to use PAW datasets[1] to accelerate calculations further.

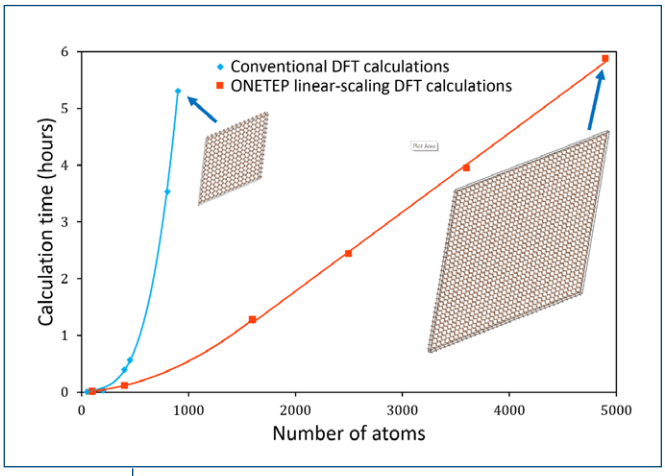


Figure 1: : ONETEP linear-scaling behavior for the calculation of the total energy of graphene segments of increasing size, compared to a conventional (cubic-scaling) DFT program. Calculations run on 160 2.0 GHz Intel Skylake cores (4 nodes, with 2x20 cores per node) with 192 GB per node.

KEY USES OF ONETEP

Insulators, Semiconductors, Glass, and Zeolites

ONETEP takes advantage of the localization of electron density and, as a consequence, finds its main application in the simulation of insulators or semiconductors. Amorphous glass surfaces and zeolites that require large unit cells to be properly described are also well-suited for ONETEP.

Catalysis

Another application for ONETEP is in the area of catalysis, where it can be used to study the influence of the support on catalytic activity. To model a support together with an active nanoparticle requires hundreds or even thousands of atoms. Therefore, a linear-scaling DFT code such as ONETEP is essential if one wants to include quantum mechanical effects in the calculation.

Nanotechnology

ONETEP opens up new possibilities in modeling nanotechnology. It can be used, for example, to study the electronic structure of carbon nanotubes for sensor applications. In particular, it can be applied to the development of biosensors, which are usually composed of a metal nanowire with antibodies attached to it. Those antibodies are selective towards a particular protein. Understanding the reactivity of the proteins requires a quantum mechanical based method, and a linear-scaling code is needed due to the sheer size of the system.

Industrial Materials

ONETEP can also provide fundamental insight into the electronic structure of materials that have important industrial applications. For example, as illustrated by the example of silicon supercells shown in Figure 2, ONETEP can model defects, fracturing and dopants. A better understanding of the properties of those materials can be translated to better performance of the final product. Modeling of this type, together with experiment, has been demonstrated to yield results at a lower cost than from experiments alone.

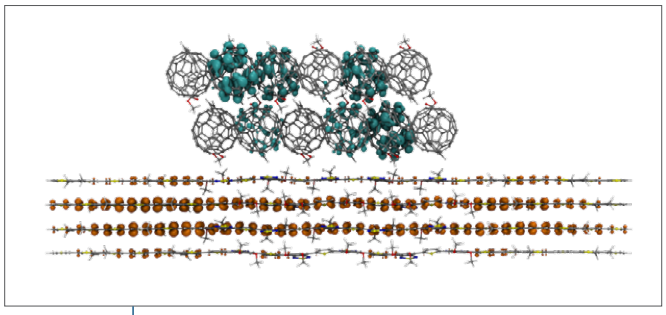


Figure 2: Charge-transfer excitation from ONETEP TDDFT calculation in a 2048-atom model of the active material (bulk heterojunction) of an organic photovoltaic[2]. The hole density (orange) is found on the polymer and the electron density (blue) is on the functionalized fullerenes. The ability to study such large structures allows more realistic simulations to be performed that capture the essential features of complex materials.

HOW DOES ONETEP WORK?

ONETEP implements DFT using the density matrix formulation. The density matrix is a quantity that is exponentially localized in insulators (and in metallic systems, at finite electronic temperature) and its diagonal elements are equal to the electronic charge density. Because the elements of the density matrix are spatially localized, the program performs many fewer calculations compared to a conventional DFT program in which the molecular orbitals are delocalized across the entire molecule.

In ONETEP, the density matrix is expressed in terms of a set of localized orbitals called non-orthogonal generalized Wannier functions (NGWFs) and a basis set of periodic sinc (psinc) functions that are equivalent to plane waves. This provides two advantages. Firstly, the basis set is easy to control with a single parameter, the kinetic energy cut-off, providing the large basis set accuracy of conventional plane-wave calculations; secondly, the NGWFs can be localized extremely well, reducing the computational effort as much as possible for the regions containing atoms while not incurring computational cost for describing regions of vacuum (e.g. vacuum above surface of material). The linear-scaling is a direct consequence of the localization of the NGWFs.

WHAT CALCULATIONS CAN ONETEP PERFORM?

The ONETEP module in BIOVIA Materials Studio allows the user to perform first-principles quantum mechanical calculations on large systems using DFT. ONETEP can currently perform the following tasks:

- Single-point energy calculation (on both insulators and metallic systems)
- Excited states (via linear-scaling time-dependent DFT)
- Geometry optimization
- Transition-state search
- Molecular dynamics
- Electron transport

Each of these calculations can be set up so that it generates specified chemical and physical properties; specifically:

- Electron density
- Bond populations
- Electrostatic potential
- Density of states (DOS), total and/or resolved by angular momentum and/or atom groups
- Mulliken charges and spins
- Molecular orbitals (MOs)

The energy of solvation of molecular or extended systems can also be calculated using a novel implicit solvation model.[3]

THE MATERIALS STUDIO ADVANTAGE TOOLS TO COMPLEMENT ONETEP

ONETEP is part of the comprehensive BIOVIA Materials Studio modeling and simulation software environment. BIOVIA Materials Studio provides a user-friendly interface that complies with Windows® standards, which together with a variety of training options, makes it easy for any user to learn the software and apply it with confidence. On top of this, BIOVIA Materials Studio offers a wealth of modeling and simulation tools that can be used to supplement ONETEP.

For example, BIOVIA Materials Visualizer — the core of BIOVIA Materials Studio — offers a wide range of model building and visualization tools that allow users to construct models of the systems of interest. In particular, researchers in nanotechnology will benefit from the nanotube builder which can create single walled, multi-walled and bundles of nanotubes, as well as the nanocluster builder, which can create spheres, tetrahedra, and other shapes. From BIOVIA Materials Visualizer, users can then easily select ONETEP to run an advanced quantum mechanics calculation.

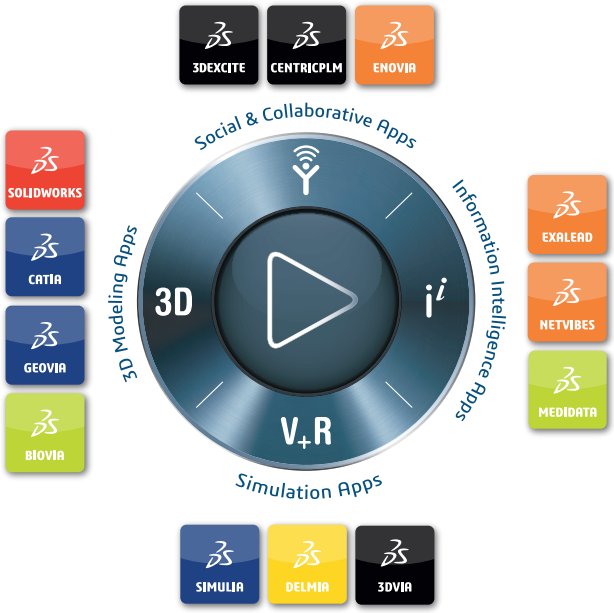
BIOVIA Materials Studio also offers analysis tools that complement ONETEP. For example, population analysis control allows the user to assign charges, spins, and bond orders derived from a Mulliken analysis to the final structure obtained in a ONETEP calculation, while other tools allow you to display 3D renderings of molecular orbitals.

On top of this, a flexible client-server architecture means that calculations can be run on servers located anywhere on a company's network. Results are returned to a user's PC, where they may be displayed and analyzed. It is easy to produce high quality graphics of molecular and materials structures, as well as molecular orbitals. Structures, graphs and other data, such as video clips, can be instantly exchanged with other PC applications, facilitating sharing among colleagues and analysis in spreadsheets or other packages.

To learn more about BIOVIA Materials Studio, go to 3dsbiovia.com/materials-studio.

REFERENCES

1. http: //www.onetep.org/Main/FAQ
2. G. Boschetto, M. Krompiec, and C.-K. Skylaris, Insights into the Charge-Transfer Mechanism of Organic Photovoltaics: Effect of Domain Size, J. Phys. Chem. C. 122, 17024 (2018).
3. J. Dziedzic, H.H. Helal, C.-K. Skylaris, A.A. Mostofi, and M.C. Payne, Minimal parameter implicit solvent model for ab initio electronic structure calculations, Europhysics Letters 95, 43001 (2011); J. C. Womack, L. Anton, J. Dziedzic, P. Hasnip, M. Probert, and C.-K. Skylaris, DL_MG: A Parallel Multigrid Poisson and Poisson-Boltzmann Solver for Electronic Structure Calculations in Vacuum and Solution, J. Chem. Theor. Comput. 14, 1412 (2018).



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