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Quantum computing  
could be game-changing  
for drug development in  
the pharmaceutical

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industry. Businesses  
should start preparing  
now.

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Pharma's digital Rx:  
Quantum computing in  
drug research and  
development

Many quantum  
mechanical (QM) and  
theory studies using  
density functional  
theory (DFT) have been  
carried out to gain

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insights into possible  
reaction intermediates  
and energy barriers  
(14–17).

Direct correlation of  
oxygen adsorption on  
platinum-electrolyte  
interfaces with the  
activity in the oxygen  
reduction reaction  
such as density  
functional theory (DFT)  
(15–19). Sampling CCS

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from scratch, even when  
done within efficient  
optimization algorithms,  
is typically an  
encyclopedical endeavor  
by nature and ignores  
the ...

Simplifying inverse  
materials design  
problems for fixed  
lattices with alchemical  
chirality

Density functional

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theory (DFT) calculations have become widely utilized in material simulations because of their remarkable ability to reproduce measured quantities. DFT calculations are limited to a ...

Modeling of Complex  
Material Systems in  
Extreme Environments

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for Space Technology

An integral part of this project is the use of density functional theory (DFT) and time-dependent DFT to understand the fluorescence quenching by metal ions and the ability of metal-ligand complexes ...

RUI: A New Paradigm  
for the Design of

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Fluorescent Anion  
Sensors

This is illustrated  
through density  
functional theory (DFT)  
calculations for the  
highest occupied  
molecular orbital/lowest  
unoccupied molecular  
orbital (HOMO/LUMO)  
energy gap and redox  
potential on ...

Reversible ketone

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functional and  
dehydrogenation for  
aqueous organic redox  
flow batteries

"Even when compared to density-functional theory (DFT), a computationally expensive and physics-informed method for crystal structure and crystalline property prediction, the ML model boasts ...

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Machine learning aids in materials design

Chiara Gattinoni, a

materials theorist and

Marie Curie Fellow at

ETH Zurich, uses the

"Piz Daint"

supercomputer at CSCS

to investigate a special

class ...

Expanding limits of

ferroelectrics

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When lithium reacts with amorphous silicon, amorphous  $\text{Li}_x\text{Si}$  is formed. The voltage composition curve of Li/a- $\text{Li}_x\text{Si}$  cells has been calculated using density functional theory (DFT) as implemented in ...

First-principles studies of the reaction of Li with amorphous Si

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In particular, by combining scanning tunneling microscopy and spectroscopy (STM and STS), inelastic electron tunneling spectroscopy (IETS), and density functional theory (DFT), the bonding in rect-v 1 ...

Synthesis of borophane polymorphs through hydrogenation of

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borophene

This phenomenon is well understood within the framework of density functional theory (DFT) - a mathematical procedure that deals with the quantum mechanics of many-electron system. Scientists ...

New approach to  
calculate electron traffic

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Mechanistic

understanding of this  
reaction has emerged

from surface science  
and density functional  
theory (DFT), but

essentially all past work  
has focused solely on  
supported palladium  
(Pd) or ...

CAREER:

Understanding Effects

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of Surface Coverage and  
Catalyst Composition  
on Vinyl Acetate  
Synthesis

The results were  
published in Chinese  
Journal of Catalysis.  
The density functional  
theory (DFT)  
calculation shows that  
the CuPd (100) interface  
enhanced the adsorption  
of CO<sub>2</sub> and reduced the

...

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Tuning reaction barriers  
for carbon dioxide  
electroreduction to

multicarbon products

Ethylene and water, two  
components present in

vehicle exhaust which  
compete for adsorption

sites are studied from

density functional

theory (DFT)

calculations. The BEEF-

vdw 2 functional is used

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in DFT...

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Trapping Properties of  
Ag/SSZ-13 Zeolite:

Modeling Adsorption  
Capacity

Over the previous decade, Dr. Becke had developed a formula to vastly improve the accuracy of chemical calculations using Density Functional Theory (DFT). But few

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were listening to him.

Now, at a ...

Axel Becke

The 25 th international  
WIEN2k workshop is a  
hands-on tutorial  
approach to teach the  
band structure  
calculations using  
Density Functional  
Theory to graduate  
students ... WIEN2k is  
one of the most ...

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Boston College

The results were  
published in Chinese

Journal of Catalysis.

The density functional  
theory (DFT)

calculation shows that  
the CuPd (100) interface  
enhanced the adsorption  
of CO<sub>2</sub> and reduced the

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