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noncovalent
interactions† Lars
Goerigk , * a Andreas
Hansen , b Christoph
Bauer , b Stephan
Ehrlich , ‡ b Asim Najibi

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a and Stefan Grimme *
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Foundations of density
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existence theorems
--Effective single-
particle equations
--Exchange-correlation
energy functional
--Virial theorems
--Orbital functionals:
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method --Time-

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dependent density

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--Relativistic density

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Series Title:

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Science Citation

Demers, Steven Brian

(2014) Advanced

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...
the applicability of a
particular
implementation of
density functional
theory to a specific
problem in materials
simulation. For those
who wish to go more
deeply into the
formalism of density
functional theory there

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are a number of reviews and books

aimed at intermediate

and advanced levels

available in the

literature [1,2,3].

Mathematical Physics

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~~Deep learning ...~~

The mechanism of the

adsorption of CO₂

onto various sites of

MgAl₂O₄ (100), in

particular with regards

to binding

coordination, was

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investigated using density functional theory (DFT) calculations. Of the available sites, CO₂ binding was calculated to be strongly adsorbed to oxygen atoms on the octahedral Al³⁺ and tetrahedral Mg²⁺ sites, with adsorption energy values of -1.60 eV and ...

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Course | Eberhard ...

Density-functional

theory (DFT) is a

computational

quantum mechanical

modelling method used

in physics, chemistry

and materials science

to investigate the

electronic structure (or

nuclear structure)

(principally the ground

state) of many-body

systems, in particular

atoms, molecules, and

the condensed

phases. Using this

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theory, the properties

of a many-electron

system can be

determined by using ...

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Steve rated it it was

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it was amazing Aug 12,

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theory guided
advances in phase-
change materials and
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Issue 10 - Wei Zhang,
Volker L. Deringer,
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Evan Ma, Matthias
Wuttig

Status and Challenges
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Theory: Trends ...

Density functional
theory (DFT) is a (in
principle exact) theory
of electronic structure,
based on the electron
density distribution
 $n(r)$, instead of the
many-electron wave
function $\Psi(r_1, r_2, r_3, \dots)$.
Having been widely
used for over 30 years

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by physicists working

on the electronic
structure of solids,
surfaces, defects, etc.,

it has more recently
also become popular
with theoretical and ...

Physics

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functional theory zoo
with the ...~~

We introduce the first
systematic database of
scanning tunneling
microscope (STM)
images obtained using
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theory (DFT) for two-dimensional (2D) materials, calculated using the Tersoff-Hamann method. It currently contains data for 716 exfoliable 2D materials. Examples of the five possible Bravais lattice types for 2D materials and their Fourier-transforms are discussed. All the ...

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Theory C. David Sherrill

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Georgia Institute of Technology. The Big Picture • DFT improves upon Hartree-Fock by including an approximate treatment of the correlated motions of electrons (these are treated in Hartree-Fock in only an averaged sense)

~~Density Functional Theory An Advanced~~
Density Functional Theory (DFT) has firmly

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established itself as the
workhorse for the
atomic-level simulation
of condensed matter
phases, pure or
composite materials
and quantum chemical
systems. The present
book is a rigorous and
detailed introduction to
the foundations up to
and including such
advanced topics as
orbital-dependent
functionals and both
time-dependent and
relativistic DFT.

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Density functional theory (DFT) constitutes a family of methodologies for quantum mechanical electronic structure calculations with broad applications to organic and main group molecules as well as more complicated systems. 1-3 These methods are of

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Theory (DFT) has firmly

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of condensed matter phases, pure or composite materials and quantum chemical systems. The present book is a rigorous and detailed introduction to the foundations up to and including such advanced topics as orbital-dependent functionals and both time-dependent and relativistic DFT.

Density functional theory — Wikipedia

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Density Functional Theory (DFT) has firmly established itself as the workhorse for the atomic-level simulation of condensed matter phases, pure or composite materials and quantum chemical systems. The present book is a rigorous and detailed introduction to the foundations up to and including such advanced topics as orbital-dependent functionals and both

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time-dependent and
relativistic DFT.

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detailed introduction to the foundations up to and including such advanced topics as orbital-dependent functionals and both time-dependent and relativistic DFT.

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thermochemistry,
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interactions. Phys.

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2017; 19 :

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Theory (DFT) has firmly

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