Hands-on Workshop and Humboldt-Kolleg: Density-Functional Theory and Beyond - Basic Principles and Modern Insights
Isfahan, Iran, May 2 - May 13, 2016

Monday, May 2: Opening and Introduction

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Walter Kohn, 1923-2016

Walter Kohn receiving an honor from Harvard in 2012.

“Physics isn’t what I do,” Walter Kohn once said. “It is what I am.”
Walter Kohn passed away April 19, 2016 at the age of 93

Number of articles and patents in materials science including the term “density functional theory” published per year during the past 25 years.

Walter Kohn at West Beach Santa Barbara at age 75

34 years before DFT invention
34 years after DFT invention
The Kohn-Sham Ansatz of Density-Functional Theory

- Kohn-Sham (1965): Replace the original many-body problem by an independent electron problem that can be solved!

\[ E_v[n] = T_s[n] + \int v(r) n(r) \, d^3r + E_{\text{Hartree}}[n] + E_{\text{xc}}[n] \]

With \( T_s[n] \) the kinetic energy functional of independent electrons, and \( E_{\text{xc}}[n] \) the unknown functional.

- The challenge is to find useful, approximate xc functionals.
To: The American Governmental Representatives

"The undersigned oppose a preventive war against Iraq without broad international support. Military operations against Iraq may indeed lead to a relatively swift victory in the short-term. But war is characterized by surprise, human loss, and unintended consequences. Even with a victory, we believe that the medical, economic, environmental, moral, spiritual, diplomatic, and legal consequences of an American preventive attack on Iraq would undermine, not protect, U.S. security and standing in the world."


signed by
41 Nobel Laureates
Physicians for Social Responsibility
and a long list of others

The US started the war on March 20, 2003, and more than ½ million people lost their lives. Peace is not in sight (from Afghanistan to Iraq to Libya).

https://player.vimeo.com/video/163726766?width=549px&height=309px&color=00ade
f&portrait=0&title=0&byline=0&autoplay=0&loop=0&player_id=vimeo-163726766

"Don’t take the easy route and say, ‘It’s just me against some huge thing.’

“You have to find the way — not huge — that you can contribute to prevent future catastrophes,”
The Novel Materials Discovery (NOMAD) Laboratory develops a Materials Encyclopedia and Big-Data Analytics tools for materials science and engineering.

Eight complementary computational materials science groups and four high-performance computer centers form the synergetic core of this Centre of Excellence.
The NOMAD Laboratory
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There are 30-40 important codes used in computational materials science.

Nomenclature, data representation, and file formats of the input and output files of these codes are different. The heterogeneity could hardly be worse.

The NoMaD Repository accepts (and requests) input and output files of all important codes. Currently, the NoMaD Repository contains 3,026,745 entries.

http://NOMAD-CoE.eu
The NOMAD Laboratory
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NoMaD Repository
https://nomad-repository.eu
also described at youtube.com

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Thanks!

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