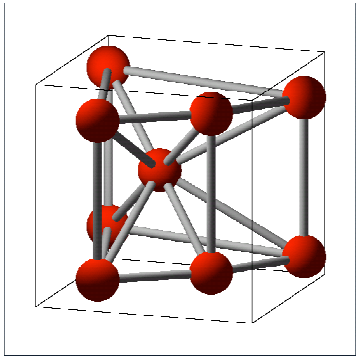
Computational Design of Strongly Correlated Materials

Sergej Savrasov

New Jersey Institute of Technology
A Public Research University

Gabriel Kotliar

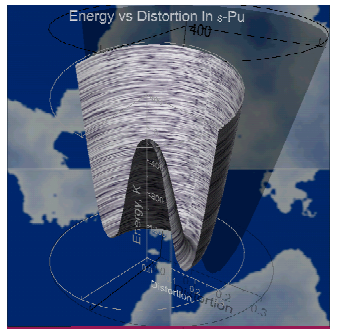
Welcome to Rutgers
The State University of New Jersey



Supported by

NSF ITR 0342290 (NJIT), 0312478 (Rutgers)

NSF CAREER 02382188 (NJIT)
NSF DMR 0096462 (Rutgers)



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Content

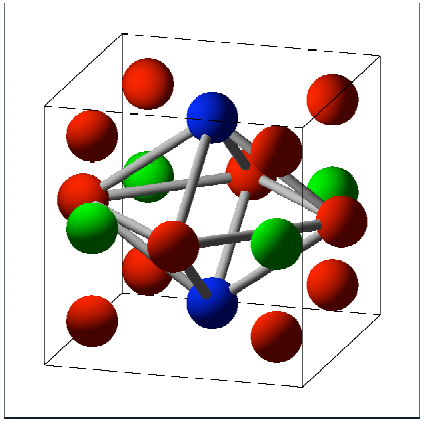
- **New Spectral Density Functional Theory to Computations of Materials**

Nature ***410***, *793 (2001), Phys. Rev. B* ***69***, *245101 (2004).*

- **Lattice Dynamics in Strongly Correlated Systems**

Phys. Rev. Lett. ***90***, *056401 (2003), Science* ***300***, *953 (2003).*

- **Material Information and Design Laboratory as ITR Tool** *http://www.physics.njit.edu/~**mindlab***



Motivation: Electronic Structure Theory of Strongly Correlated Systems

Whole range of phenomena is not accessible by LDA calculations:
excitational spectra of **strongly correlated systems,**
atomic magnetism, heavy fermions, systems near Mott transition, etc.

LDA total energies are not accurate as well.

- Properties of transition metal oxides:

No access to paramagnetic insulating regime.
Wrong phonon spectra.

- Properties of materials across lanthanide and actinide series

Well-known examples are volume collapse transitions (Ce, Pu, Pr, Am)

Merging **many-body** approaches with **electronic structure**
is needed. The well-known example is perturbative GW method.

Electronic Structure Calculations with Dynamical Mean Field Theory

Dynamical Mean Filed Theory is a non-perturbative many-body method which recognizes local correlation effects. It works self-consistently for all ratios of bandwidth W to local Coulomb interaction U.

Integration of advances: density functional electronic structure and many-body DMFT.

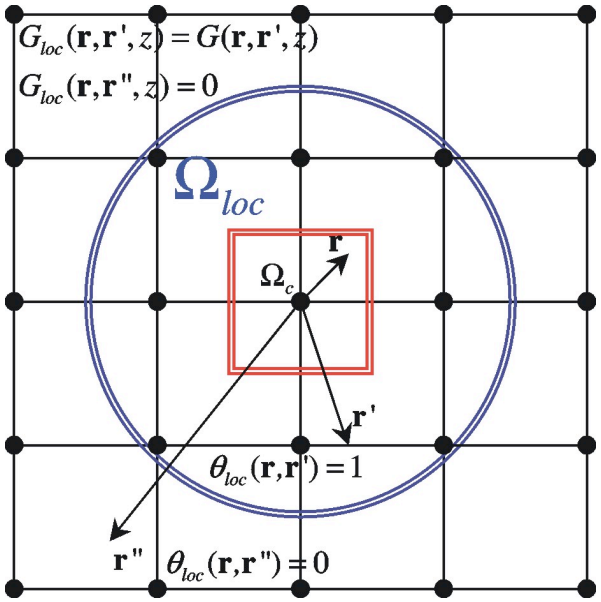
Anisimov, Poteryaev, Korotin, Anokhin, Kotliar, J. Phys. Cond. Mat. 35, 7359 (1997), A Lichtenstein, M. Katsnelson, Phys. Rev. B 57 6884 (1998)

Significant progress due to recent series of publications by the groups from IMF Ekaterinburg, University of Augsburg, LLNL Livermore, ENS, Paris, University of Nijmegen, Rutgers Piscataway etc.

Savrasov,Kotliar, Abrahams, full self-consistent implementation of LDA+DMFT Nature **410**, 793 (2001).

Computation of Materials: Functional Approach

Family of Functionals



Spectral Density Functional Theory

*[Savrasov, Kotliar, Abrahams, Nature **410**, 793 (2001),*
*Savrasov, Kotliar, Phys. Rev. B **69**, 245101 (2004)]*

• SDFT considers total energy as a functional of local Green function

• **Total Energy** is accessed similar to DFT.

• **Local excitational spectrum** is accessed.

• Good approximation to exchange-correlation functional is provided by **local dynamical mean field theory**.

• Role of Kohn-Sham potential is played by a **manifestly local** self-energy operator $M(r,r',\omega)$.

• **Generalized Kohn Sham equations** for continuous distribution of spectral weight to be solved self-consistently.

Features of Spectral Density Functional

Mott metal insulator tranisition, atomic limit are built-in into the **spectral density functional.** Larger class of problems can be studied. (phase diagrams, magnetic ordering temperatures, Kondo effect, etc)

Spectral density functional is formally *ab initio*, Coulomb interaction parameters such as **U** can be determined self-consistently within the method. (*Kotliar+Savrasov, 2001, Sun+Kotliar, PRB 2002, Zein+Antropov PRL 2002, George+Ferdi+Bierman, PRL 2002)*

- Applications to models have been done using GW+EDMFT (*Sun+Kotliar, PRB 2002, PRL 2004)*
- Applications to materials are restricted to so called **LDA+DMFT** approximation.

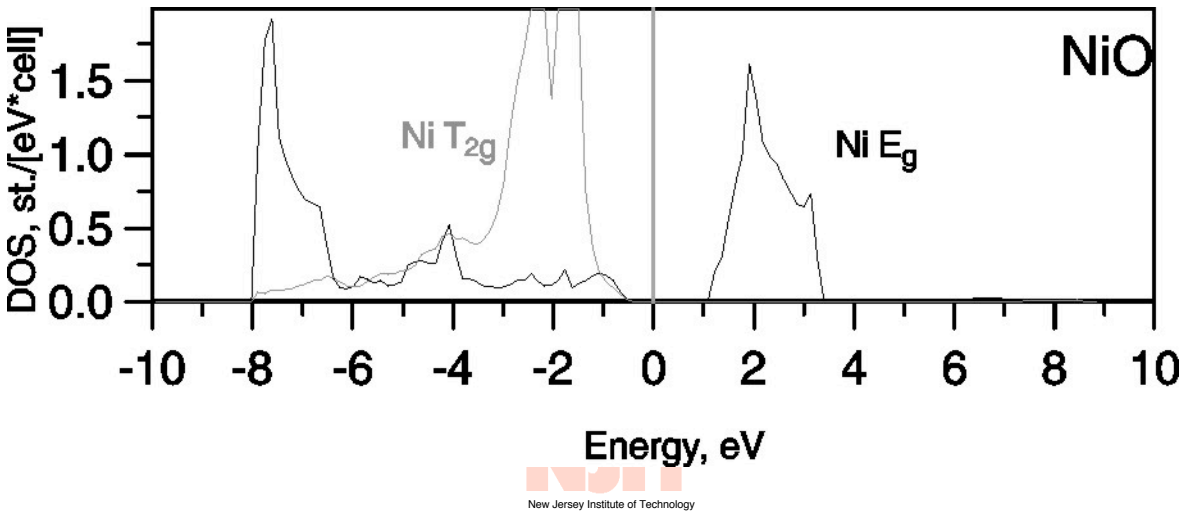
Spectral density functional provides foundation for studying **lattice dynamics** of strongly correlated systems *(Savrasov+Kotliar, PRL 2003)*

Studies of Transition Metal Oxides

θ NiO, MnO are classical Mott-Hubbard insulators. LDA (LSDA, LSDA+U) works for magnetically ordered phases only.

θ Paramagnetic regime cannot be accessed by LDA which would give a metal.

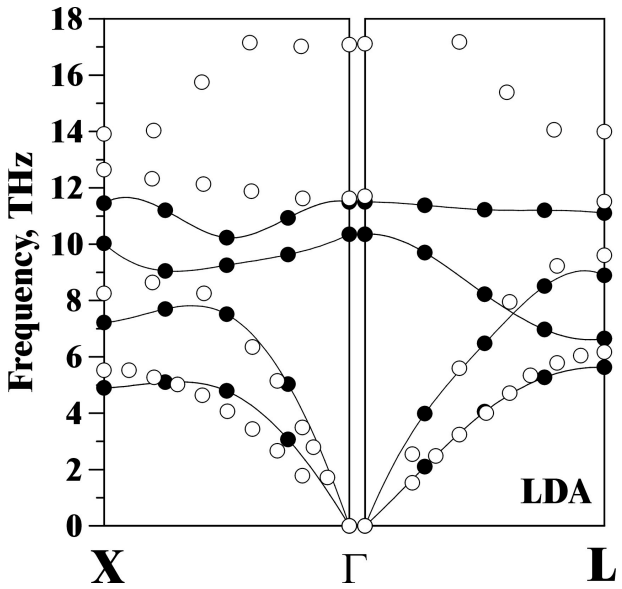
θ **Paramagnetic Mott insulator is recovered by LDA+DMFT**



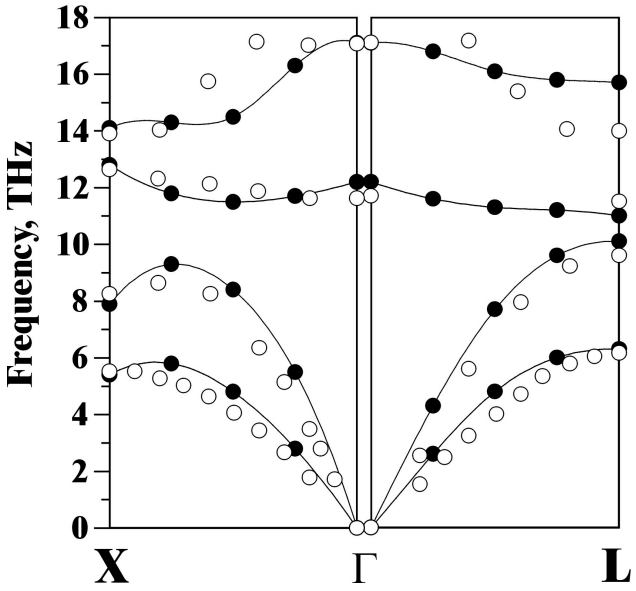
NiO: Phonons in LSDA vs. LDA+DMFT

Solid circles – theory, open circles – exp. (*Roy et.al, 1976*)

LSDA, AFM phase

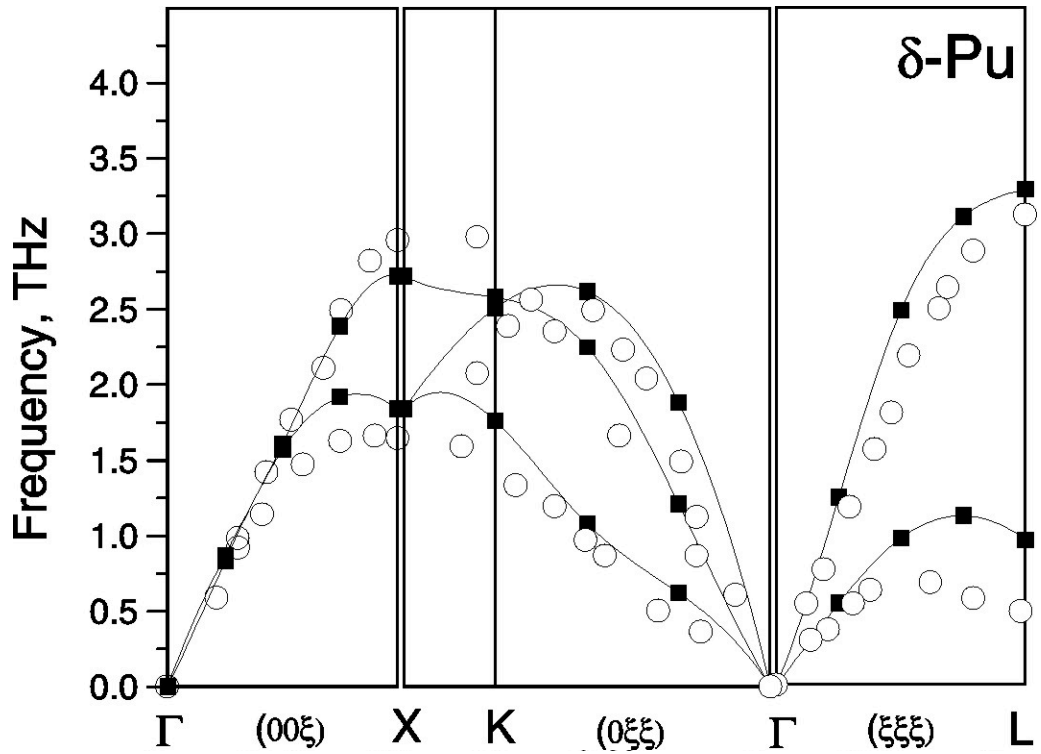


LDA+DMFT, PM phase



(after Savrasov, Kotliar, PRL 2003)

Phonons in δ-Pu



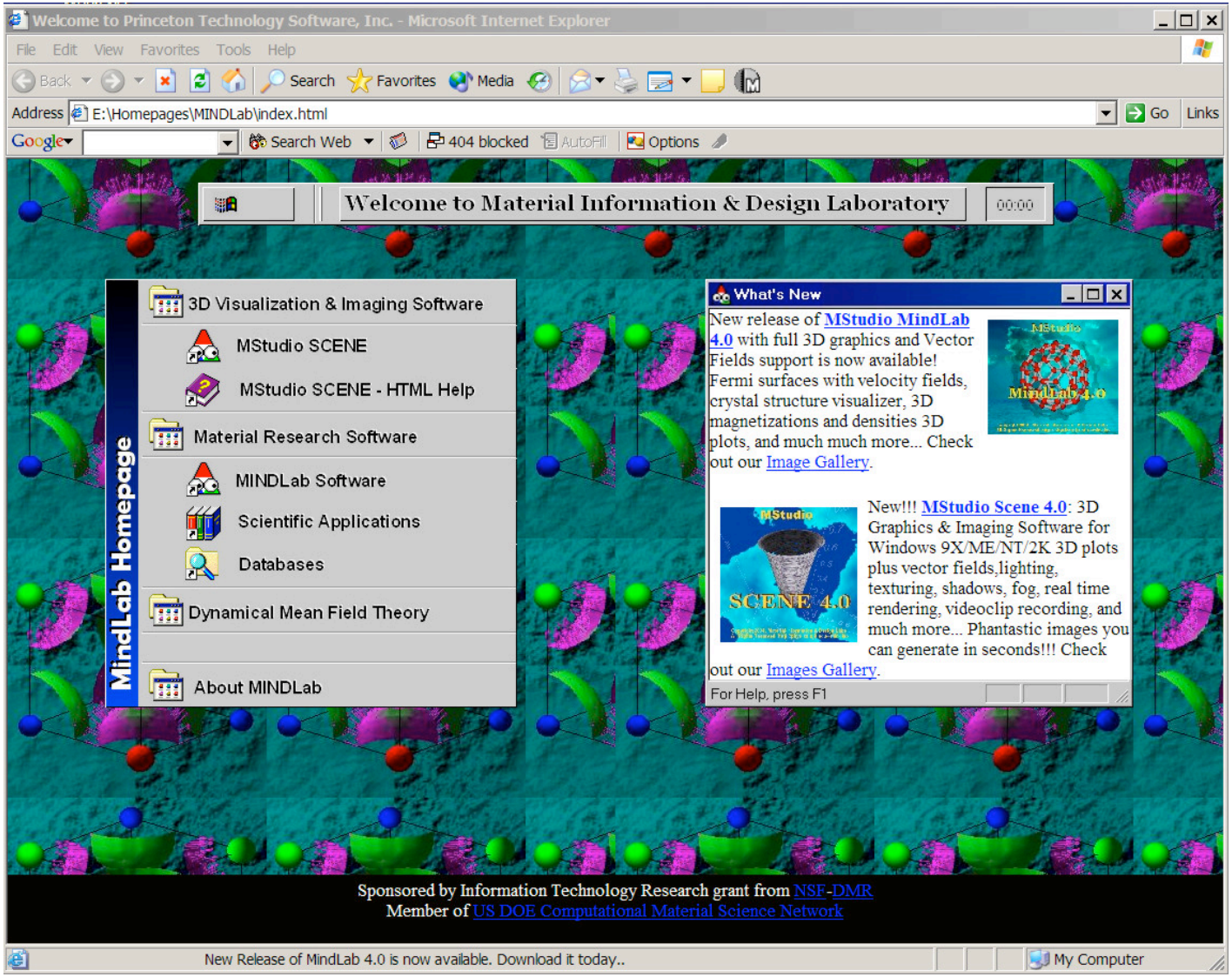
	C_{11} (GPa)	C_{44} (GPa)	C_{12} (GPa)	C'(GPa)
Theory	34.56	33.03	26.81	3.88
Experiment	36.28	33.59	26.73	4.78

(after Dai, Savrasov, Kotliar,Ledbetter, Migliori, Abrahams, Science, 9 May 2003)

(experiments from Wong et.al, Science, 22 August 2003)

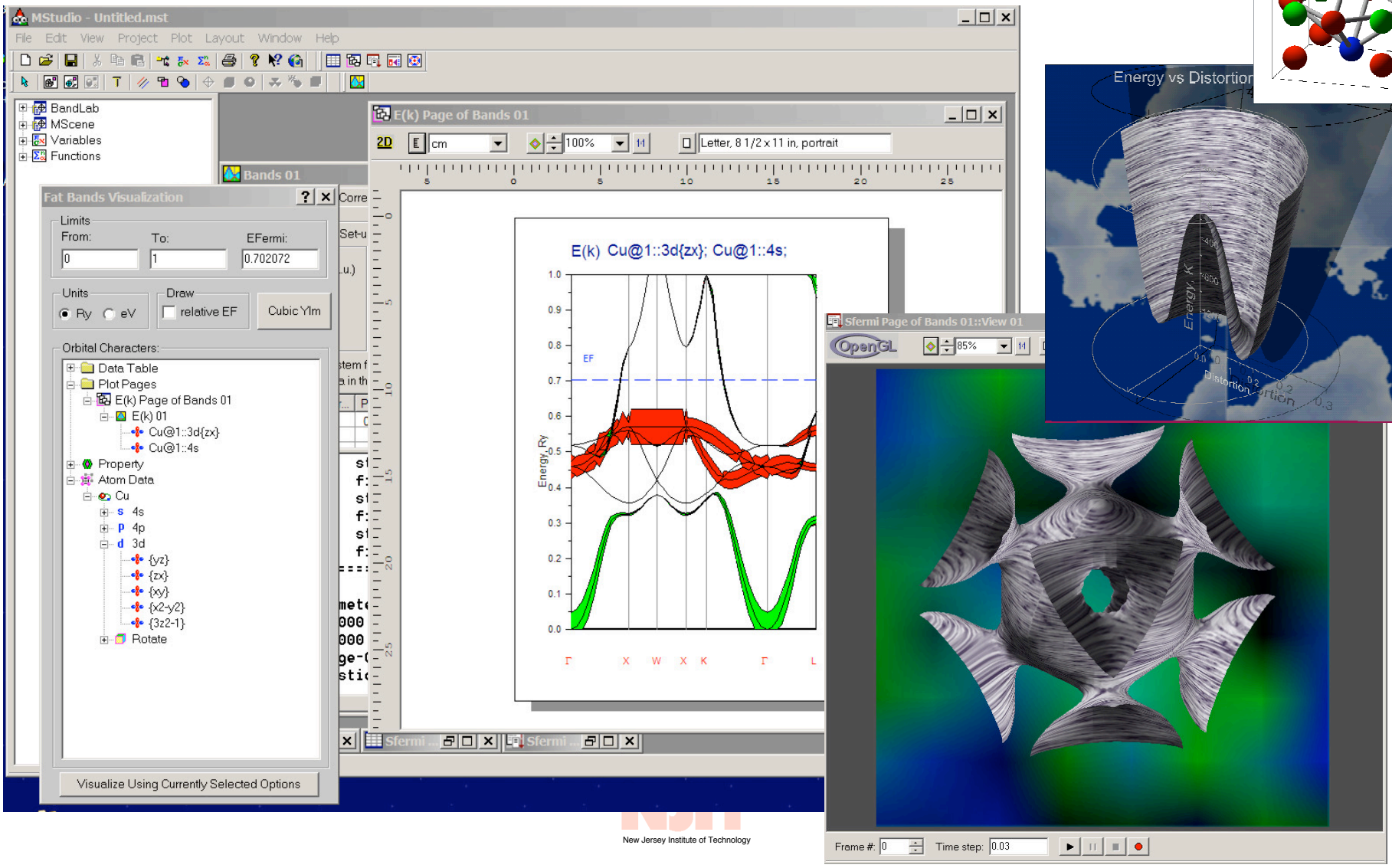
Material Information and Design Laboratory

http://www.physics.njit.edu/~mindlab



MINDLab Software: ITR Tool to Study Materials

http://www.physics.njit.edu/~mindlab



New Jersey Institute of Technology

Material Research Database

http://www.physics.njit.edu/~mindlab

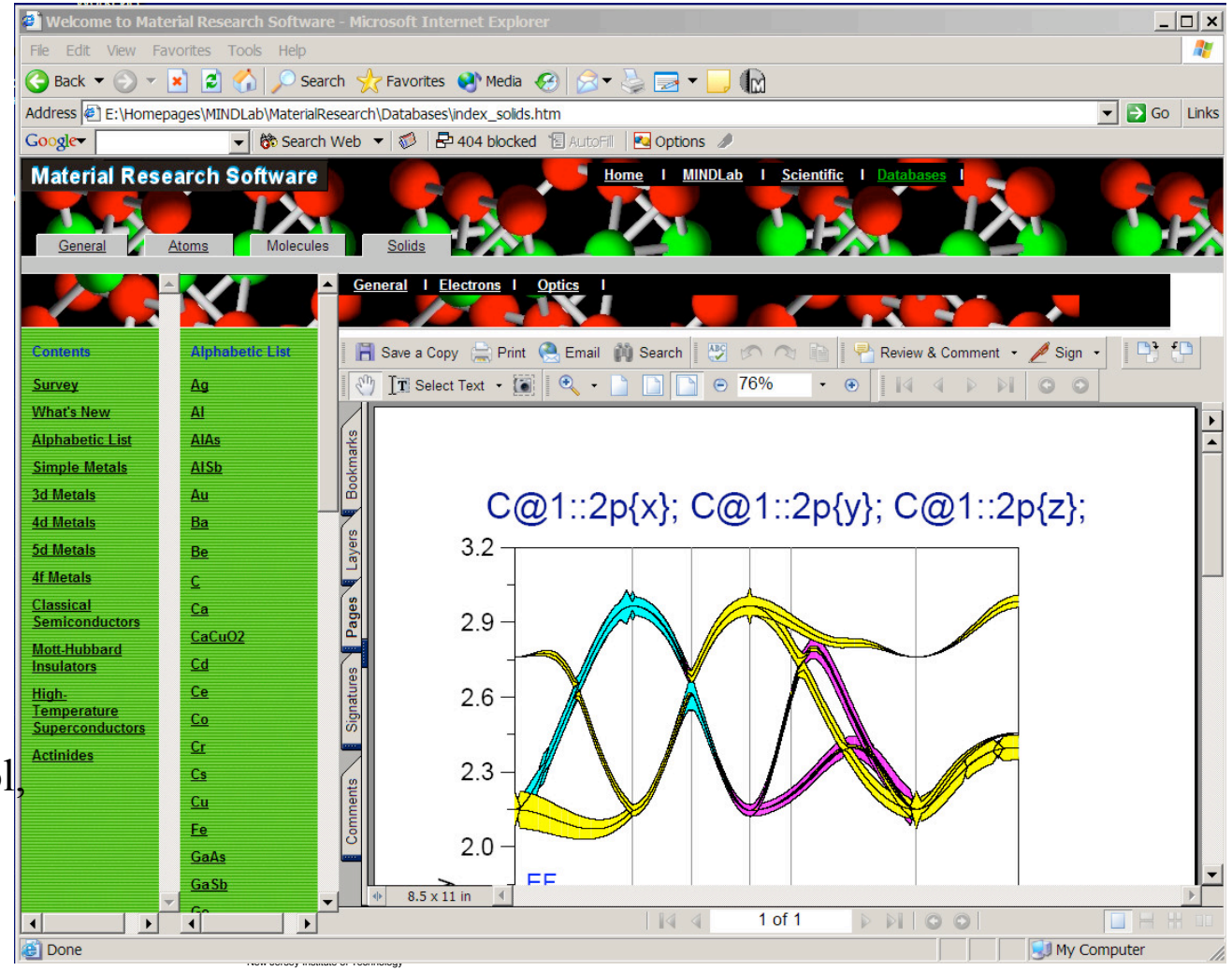
Contributions from high school students:

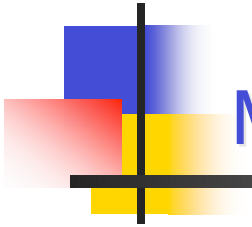
Jorge Supelano,
High Tech High School.
Summer 2001.

Julius Johnson,
Bloomfield High School,
Summer 2002.

Seung Choi,
Bloomfield High School,
Summer 2003.

Tao Lin,
Newark Central High School,
Summer 2004.





MINDLab Project

NJIT Team:

S. Savrasov
X. Nie (postdoc supported by NSF ITR)
Q. Yin (PhD student supported by NSF CAREER)

Rutgers Team:

G. Kotliar
P. Sun (postdoc supported by NSF ITR) presenting a poster.