The Abdus Salam
International Centre for Theoretical Physics

United Nations
Educational, Scientific and
Cultural Organization

IAEA
International Atomic Energy Agency

2137-13

Joint ICTP-IAEA Advanced Workshop on Multi-Scale Modelling for Characterization and Basic Understanding of Radiation Damage Mechanisms in Materials

12 - 23 April 2010

Electronic structure of UO2

J.J. Kohanoff
The Queen's University of Belfast
United Kingdom

Electronic structure of UO_2

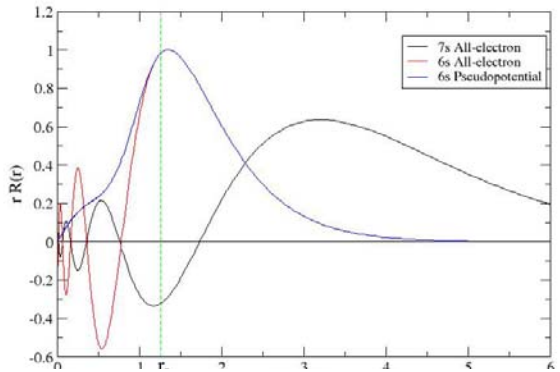
Using the quantum-espresso package (http://www.quantum-espresso.org/)

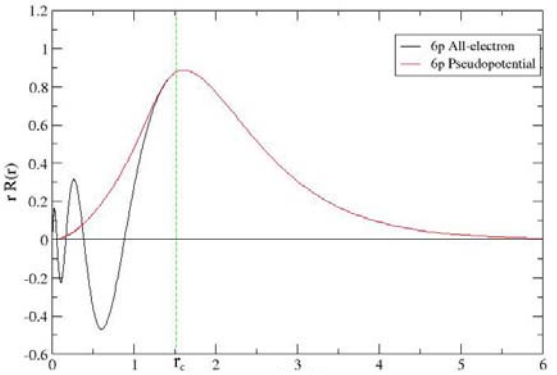
- Pseudopotentials
- Plane wave basis set

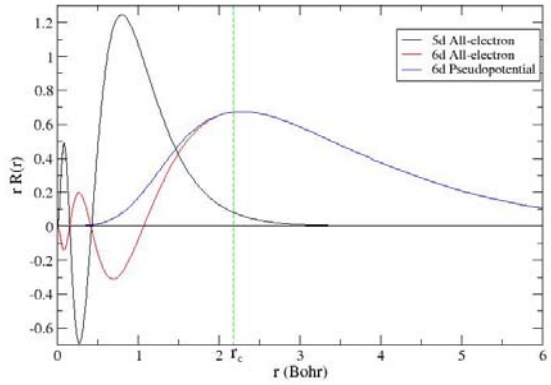
Properties

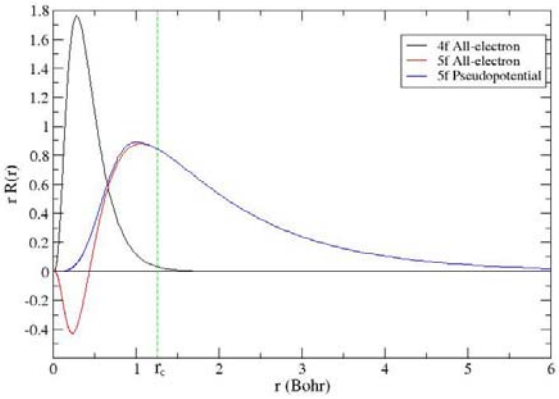
- fluorite structure
- fcc, 3 atoms un unit cell
- Lattice constant = 10.26 Bohr
- Electronic insulator. E_g=2.1 eV
- Electronic configuration of U: $[Rn]7s^2 6d^1 5f^3$
- U^{4+}: f^2
- 5f-band partially occupied (2/7)
- UO_2: splitted by crystal field: $t_{1u}(3)+t_{2u}(3)+a_g(1)$
- Still partially occupied (2/3)
- Jahn-Teller distortion opens gap.

Pseudopotential

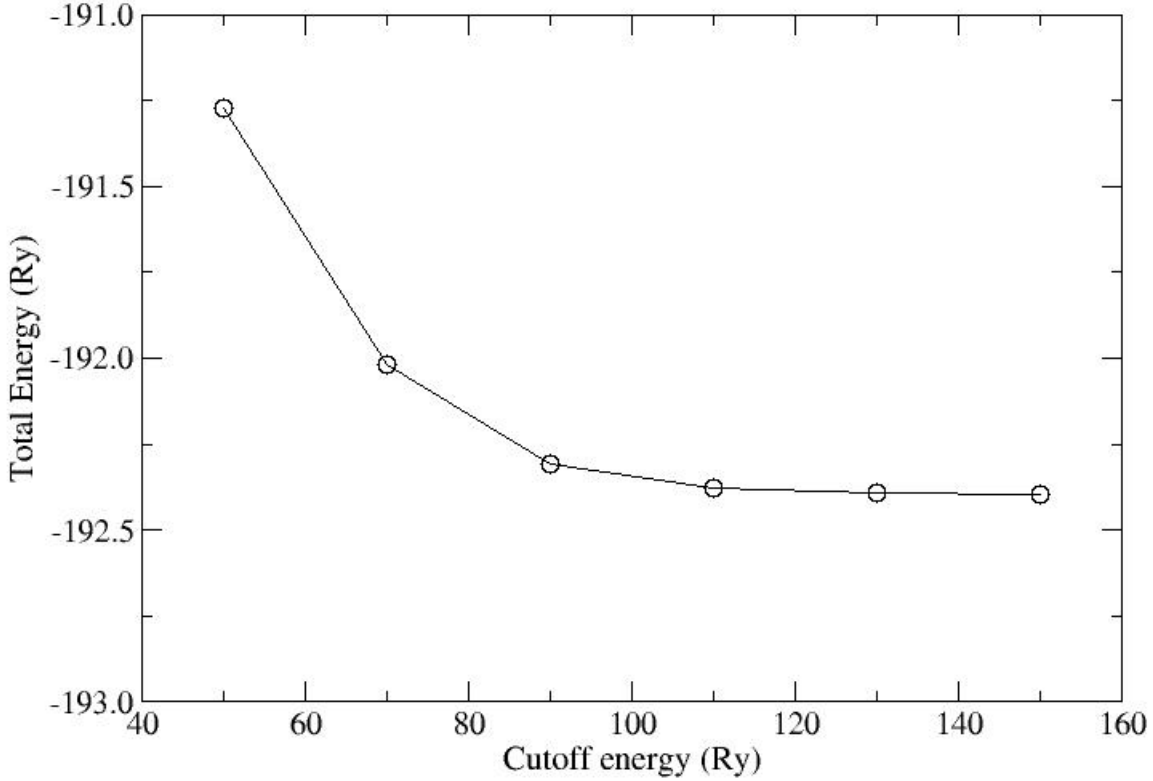




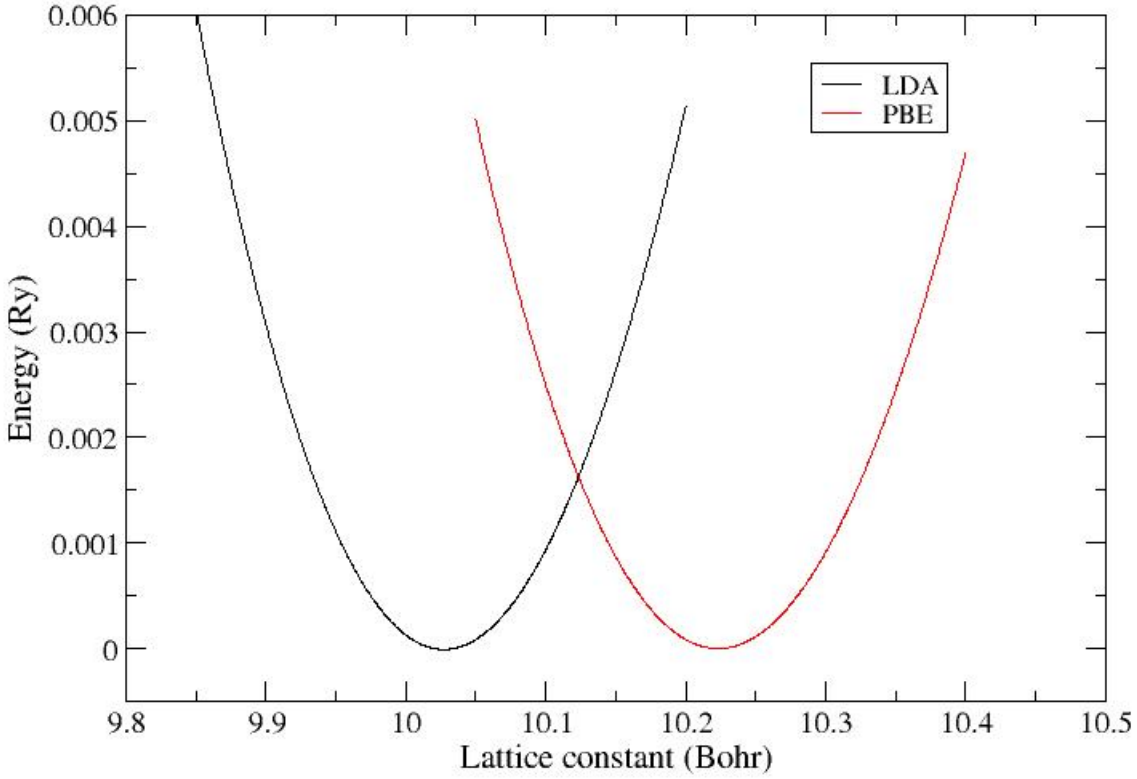




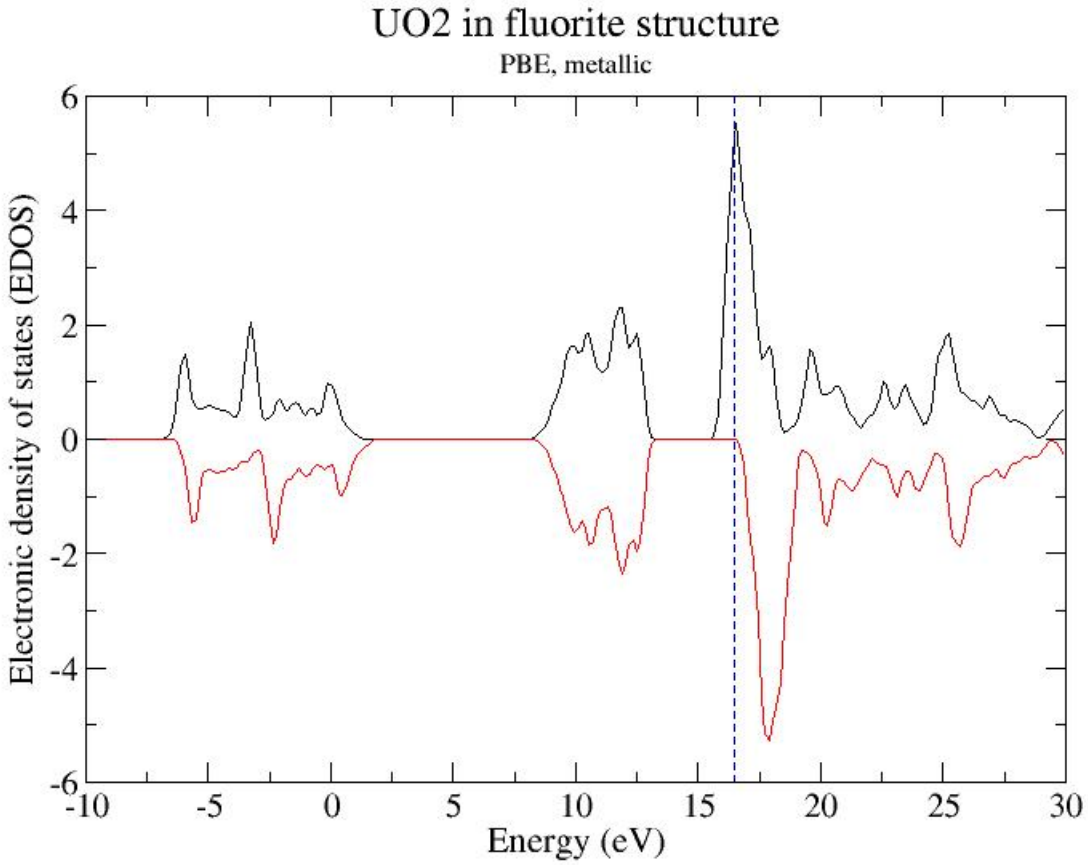
Convergence with basis set size



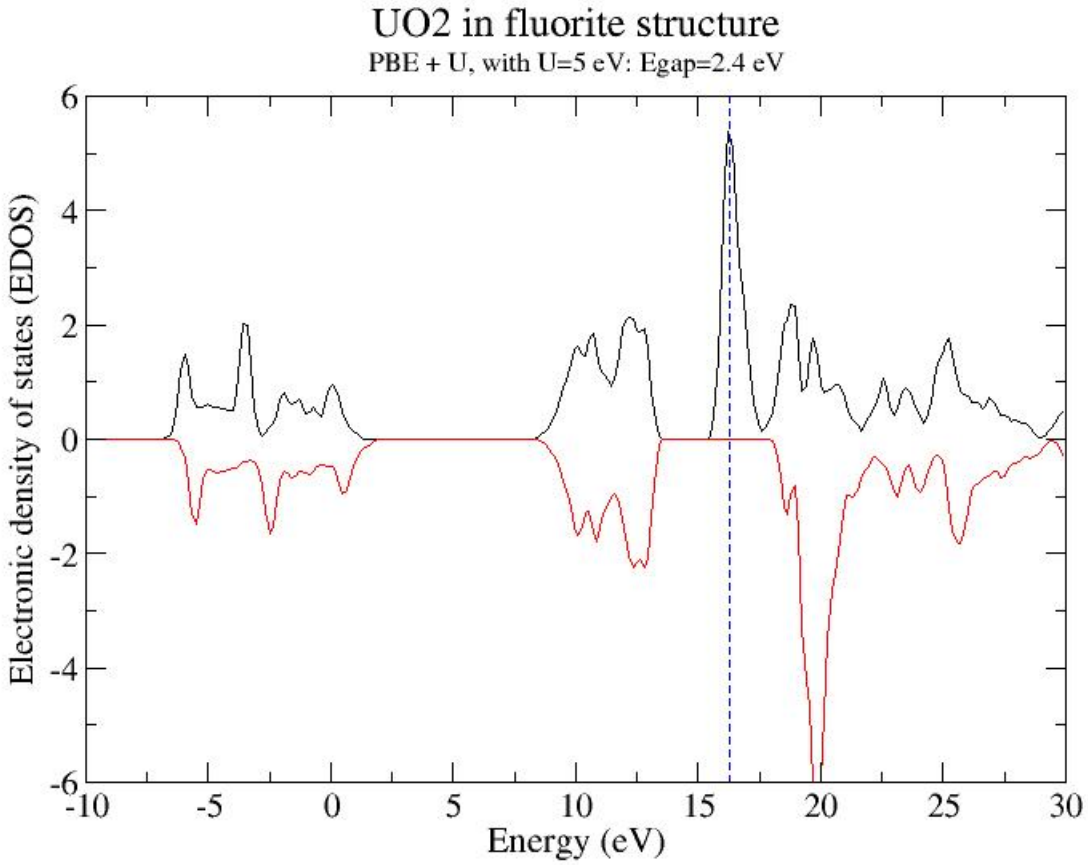
Energy-volume curve



GGA(PBE) density of states



GGA+U density of states



GGA+U density of states distorted