Physical mechanism of bioluminescence

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The talk with Prof O. Shimomura of 3rd Sept.
& our report at the Conference
«Bioluminescent Biotechnologies»,
Krasnoyarsk, SibFU of 6th Sept. 2013

Let’s ask the Google:
"Physical mechanism of bioluminescence"

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Some preliminary notes

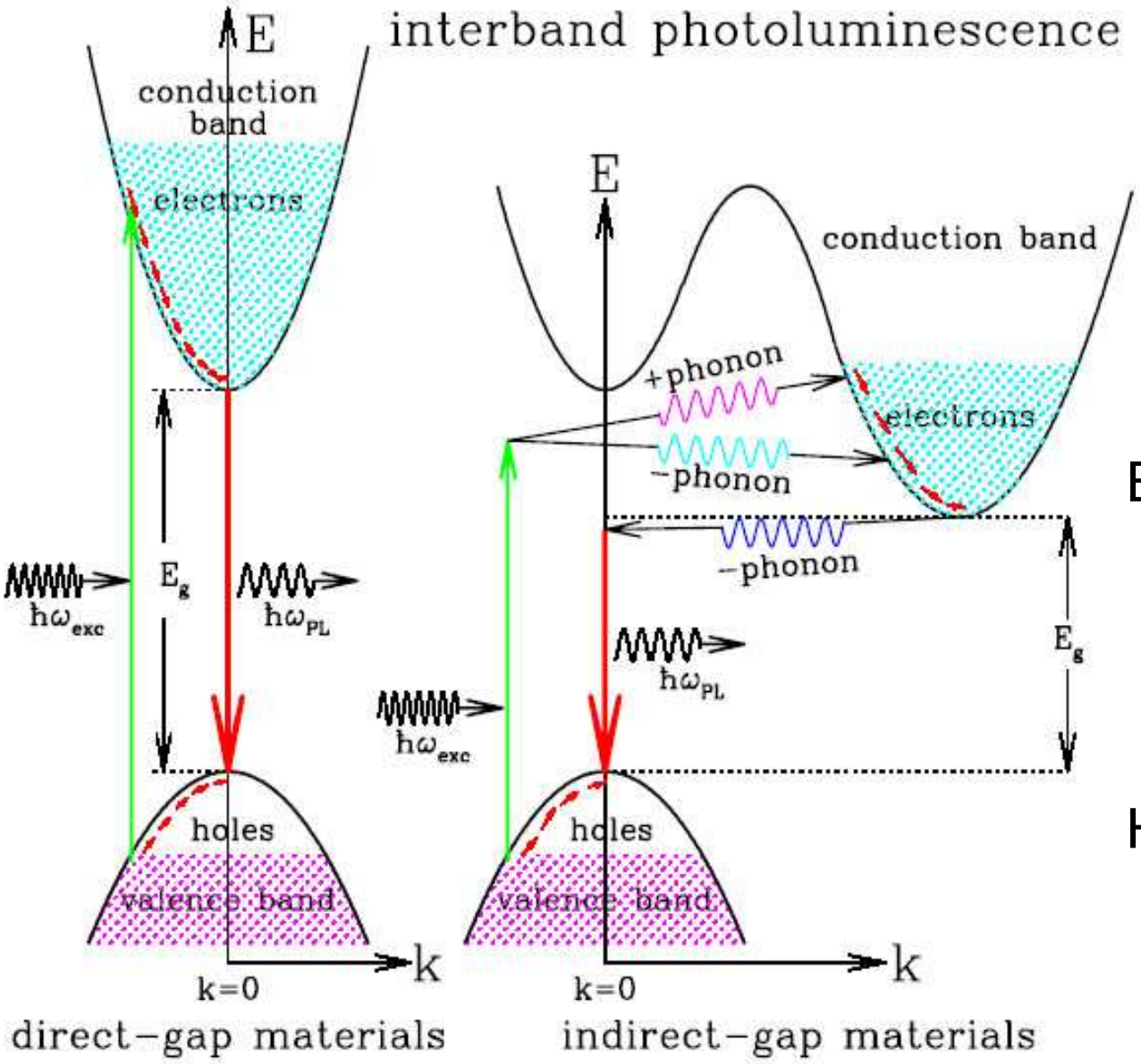
- One of us tries to understand the mist more than a quarter century:
  - Belobrov P.I. Physical mechanism of bioluminescence // *J.Biolum. Chemilum*, **2** (4), 181 (1988).
- He defends the statement (1997):
- "The physical mechanism of bioluminescence is the charge separation in the chemical excitation of the supramolecular structure of the protein“.
- Now we are thinking:
- "Physical mechanism of bioluminescence is the band gap formation in the collective electronic states of an emitting center“.

Physical Mechanism of Bacterial Bioluminescence

- http://web.mit.edu/nelman/Public/Noel_Elman_PhD_Thesis.pdf
- Noel M. Elman. Heterodyne Detection of Optical Bioreporters Based on Micro-Opto-Electro-Mechanical-Systems (MOEMS) Methods // PhD Thesis, Tel Aviv Uni., 2006. 199 p.
  - 2.2.4. Physical Mechanism of Bioluminescence

- There is more about (1997, докт.дис. ПИ):
  - 6.3. Физический механизм биолюминесценции

Mechanism of (bio)luminescence



"Bio" prefix could be misleading: luminescence is described in crystalline materials in terms of interband electron transitions. Dispersion is important.

Band theory cannot be used for aperiodic systems: liquids, luminescent protein in water environment, etc.

However, relatively large supercell allows to apply band theory even to aperiodic materials

"Band structure" of aperiodic systems: liquid water

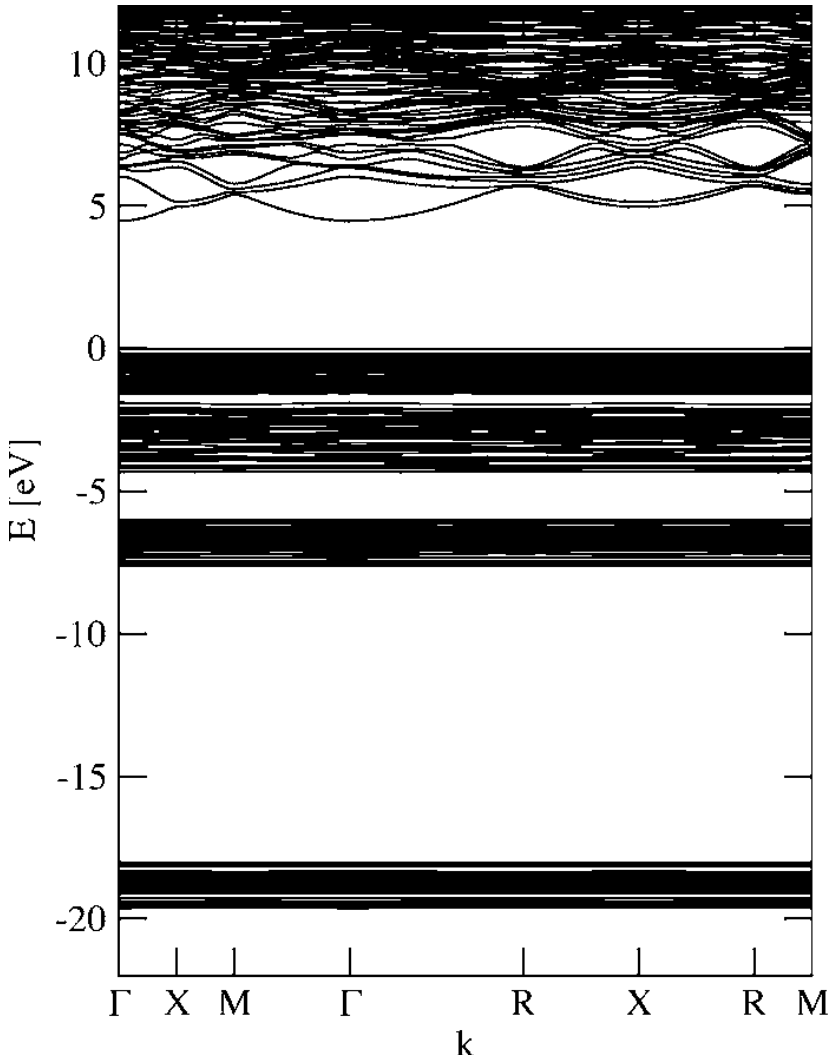
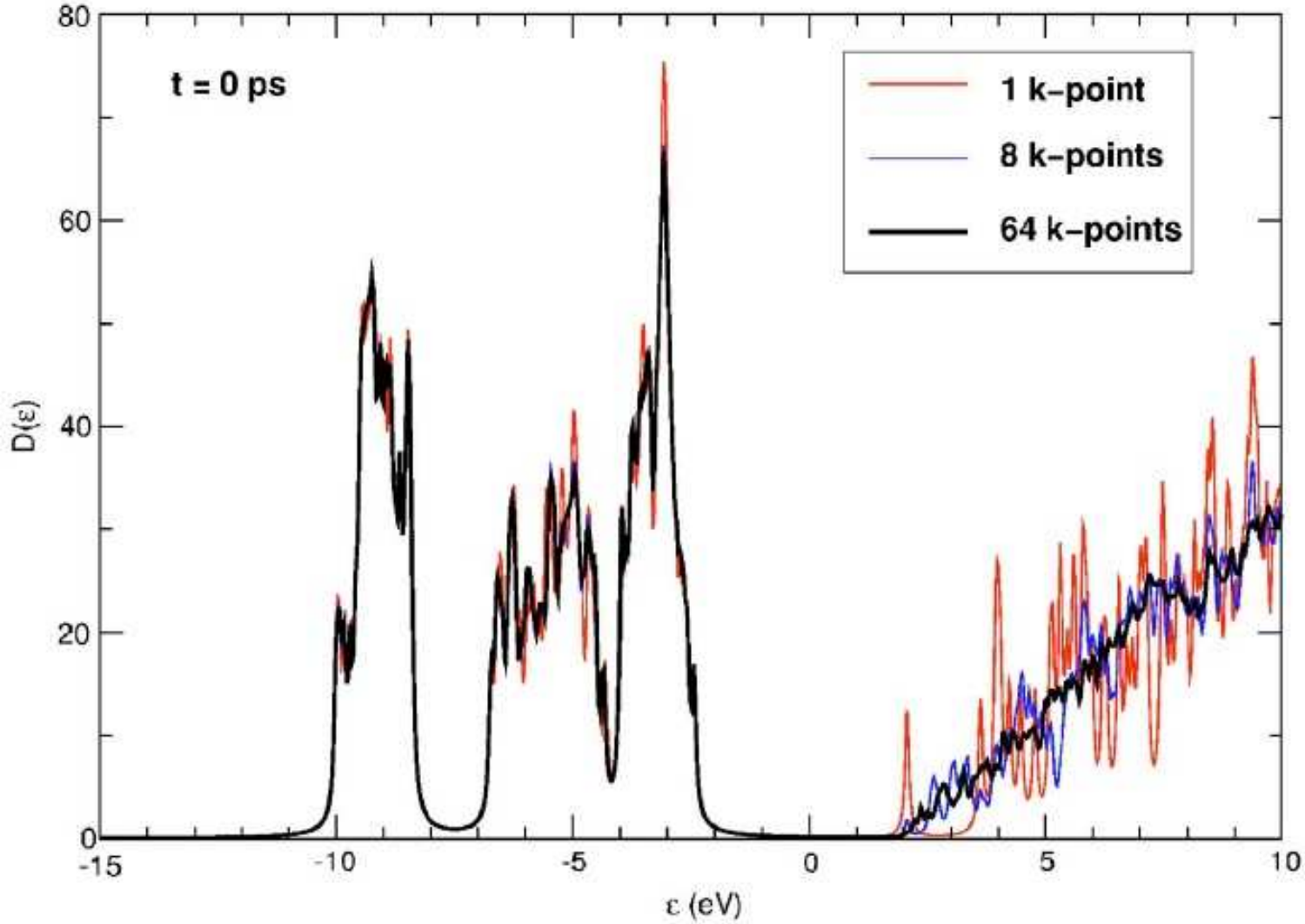


Fig.6. Computed DFT/PBE “band structure” for one representative 32-molecule supercell of liquid water taken from a TIP4P trajectory. The electronic charge density is converged using the Γ point only.

- Conduction band dispersion is significant!
- Valence band energy has almost no dispersion: no need in k-space sampling
- Overall: dispersion should be taken into account when considering luminescent molecules in water matrix

D Prendergast, J D Grossman, G Galli // *J Chem Phys* **123** (1), 14501 (2005).

Correct DoS of liquid water



- Separate peak (red) occurs near the bottom of the conduction band and then disappears as number of k-points is increased
- k-point sampling is vital for correct conduction band description!

D Prendergast, J D Grossman, G Galli // *J Chem Phys* **123** (1), 14501 (2005).

Towards exact physical mechanism of bioluminescence

Now we plan to develop the statement:

- the charge separation in the chemical excitation of the supramolecular structure of the protein (Luciferase)

together with:

- the band gap formation in the collective electronic states of joint emitting center: protein, cofactor & water.