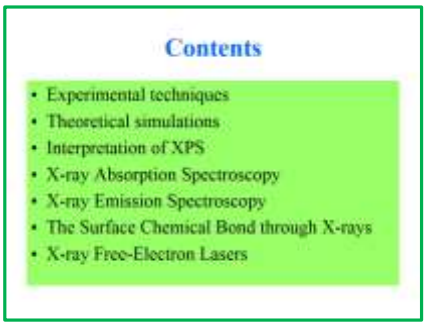
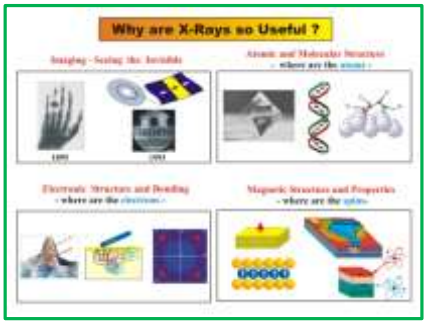
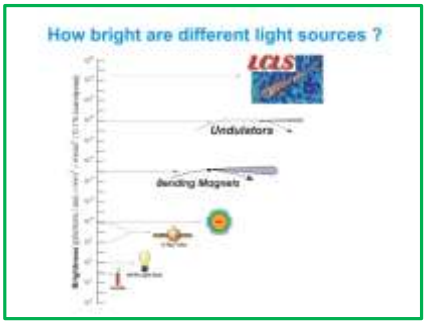
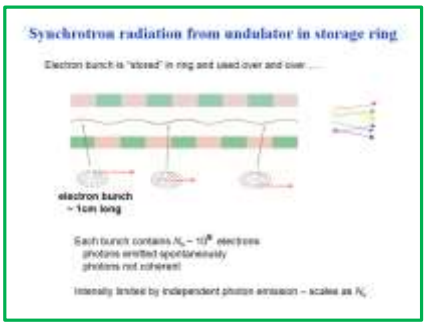
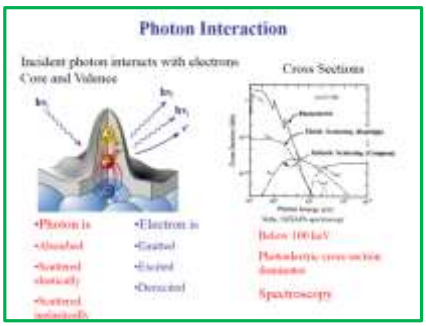
"НА КОКТЕЙЛ ОТ ЗНАНИЯ"





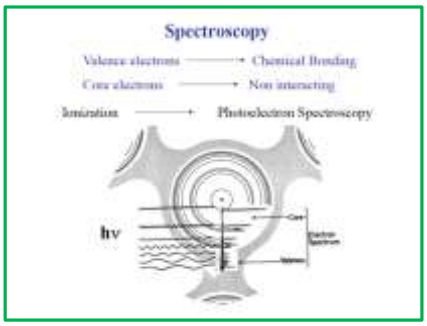


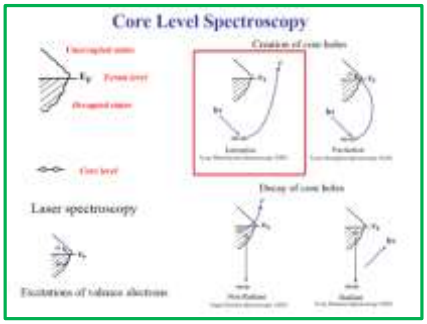


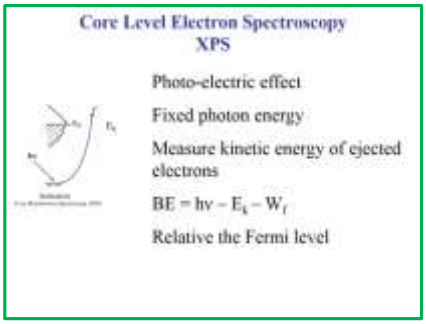


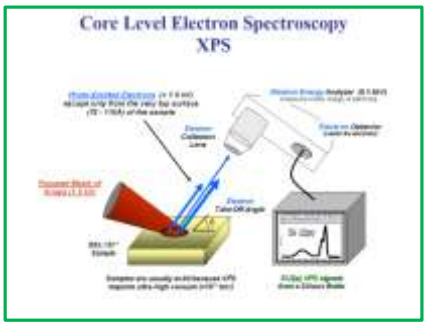
Проект BG05M2OP001-2.009-0028 "Постигане на оптимална среда за обучение, научни изследвания, иновации и устойчиво развитие на човешкия капитал в сферата на химическите науки: Адаптиране на образованието днес за утрешния ден", финансиран от Оперативна програма „Наука и образование за интелигентен растеж“, съфинансирана от Европейския съюз чрез Европейските структурни и инвестиционни фондове.

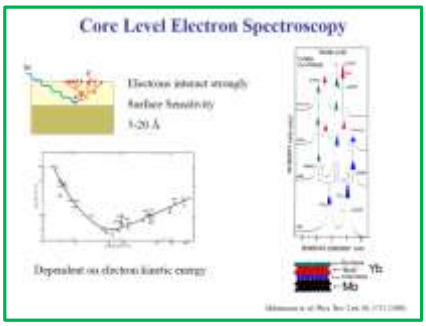
"НА КОКТЕЙЛ ОТ ЗНАНИЯ"

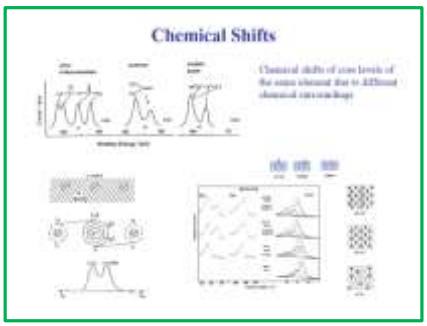


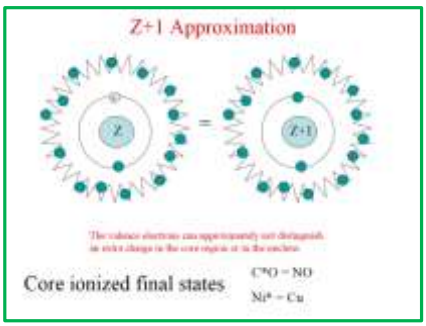






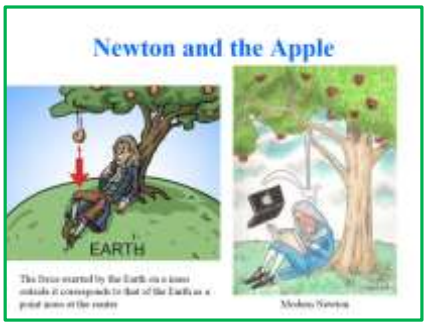


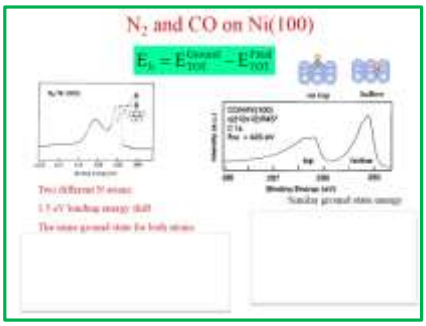


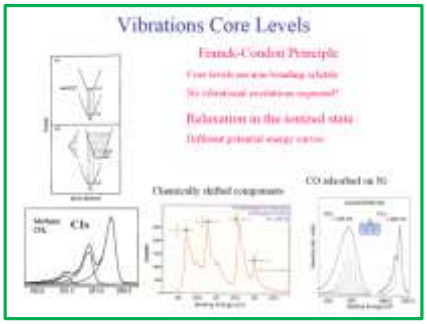


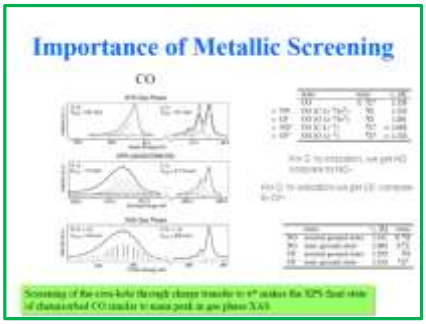
Проект BG05M2OP001-2.009-0028 "Постигане на оптимална среда за обучение, научни изследвания, иновации и устойчиво развитие на човешкия капитал в сферата на химическите науки: Адаптиране на образованието днес за утрешния ден", финансиран от Оперативна програма „Наука и образование за интелигентен растеж“, съфинансирана от Европейския съюз чрез Европейските структурни и инвестиционни фондове.

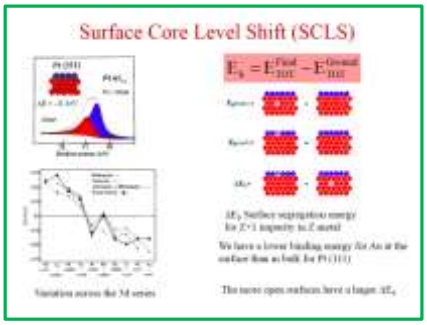
"НА КОКТЕЙЛ ОТ ЗНАНИЯ"

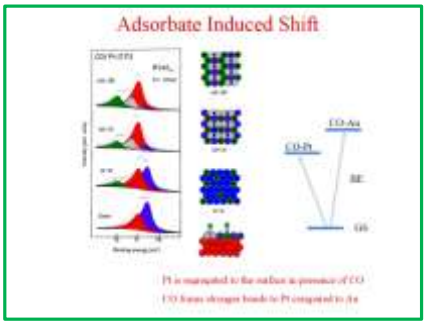


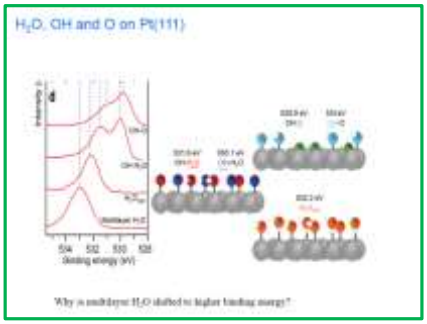


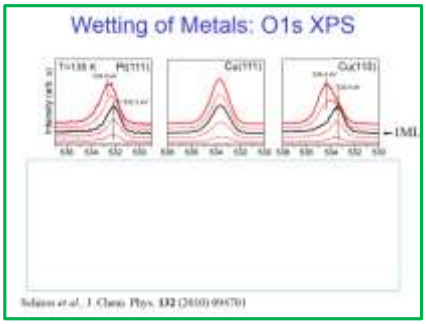






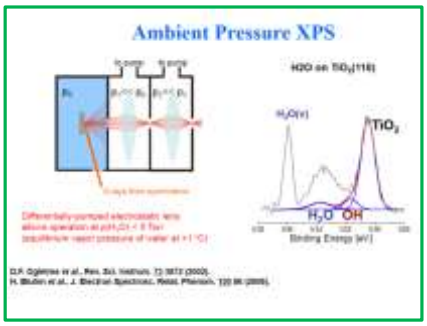


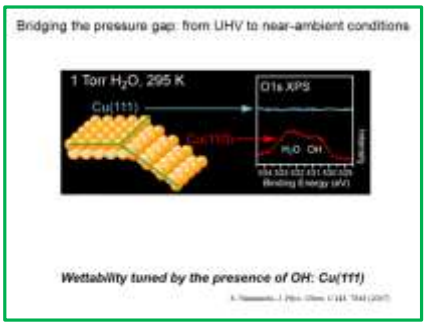


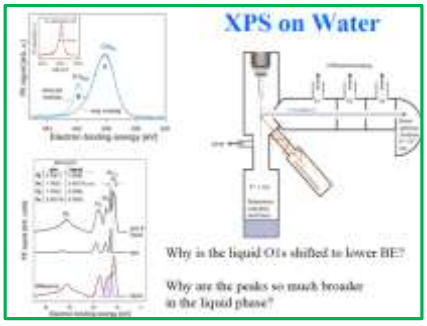


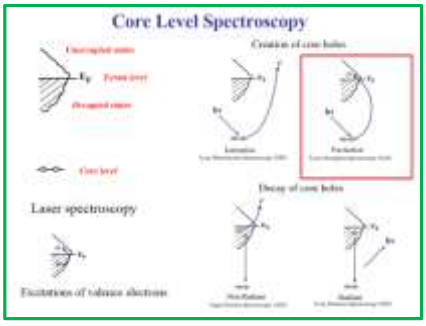
Проект BG05M2OP001-2.009-0028 "Постигане на оптимална среда за обучение, научни изследвания, иновации и устойчиво развитие на човешкия капитал в сферата на химическите науки: Адаптиране на образованието днес за утрешния ден", финансиран от Оперативна програма „Наука и образование за интелигентен растеж“, съфинансирана от Европейския съюз чрез Европейските структурни и инвестиционни фондове.

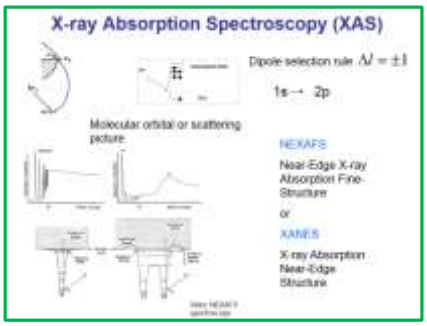
"НА КОКТЕЙЛ ОТ ЗНАНИЯ"

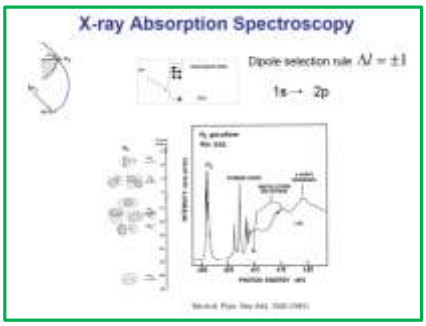


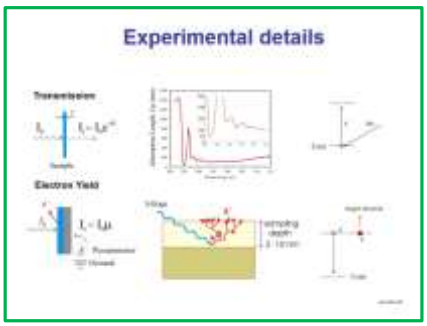


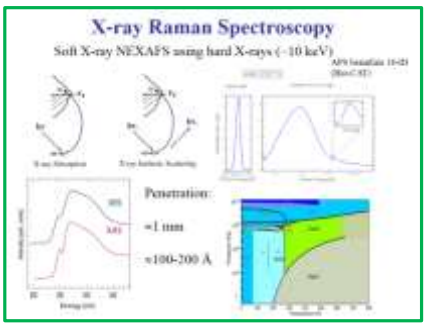






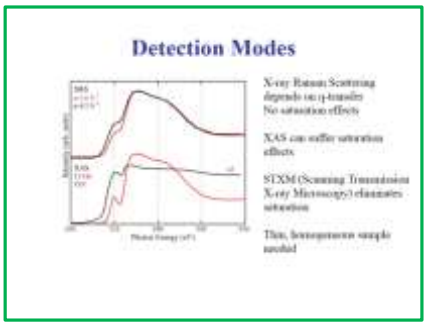


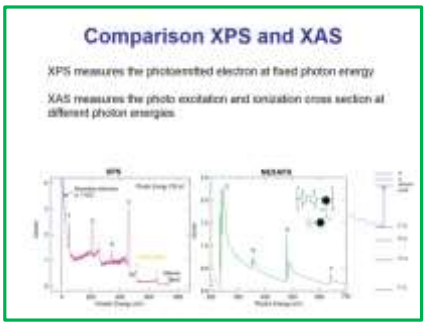


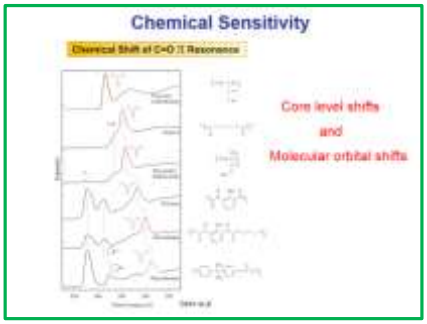


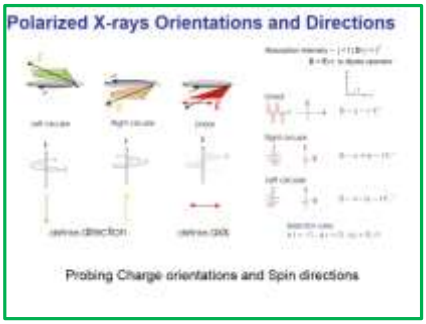
Проект BG05M2OP001-2.009-0028 "Постигане на оптимална среда за обучение, научни изследвания, иновации и устойчиво развитие на човешкия капитал в сферата на химическите науки: Адаптиране на образованието днес за утрешния ден", финансиран от Оперативна програма „Наука и образование за интелигентен растеж“, съфинансирана от Европейския съюз чрез Европейските структурни и инвестиционни фондове.

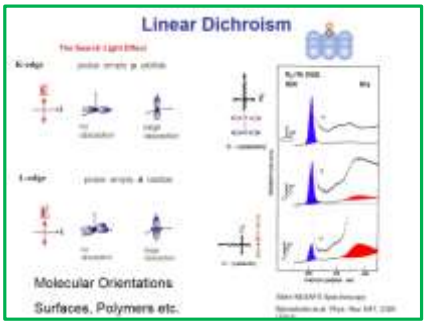
"НА КОКТЕЙЛ ОТ ЗНАНИЯ"

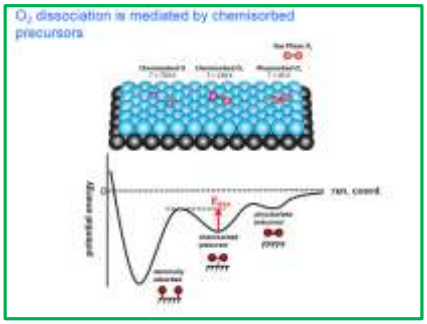


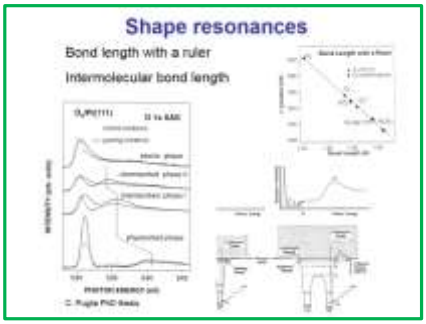






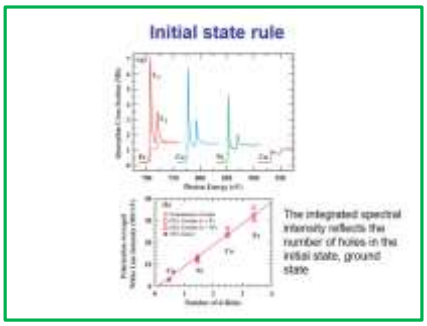


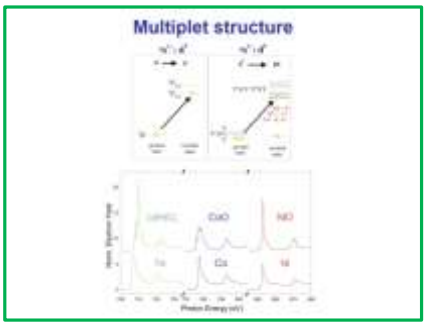


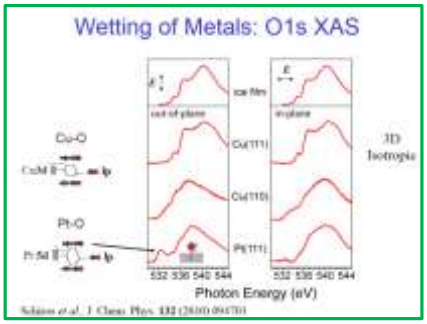


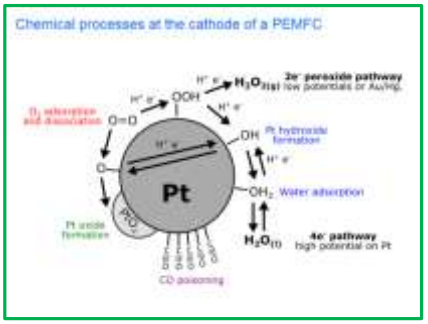
Проект BG05M2OP001-2.009-0028 "Постигане на оптимална среда за обучение, научни изследвания, иновации и устойчиво развитие на човешкия капитал в сферата на химическите науки: Адаптиране на образованието днес за утрешния ден", финансиран от Оперативна програма „Наука и образование за интелигентен растеж“, съфинансирана от Европейския съюз чрез Европейските структурни и инвестиционни фондове.

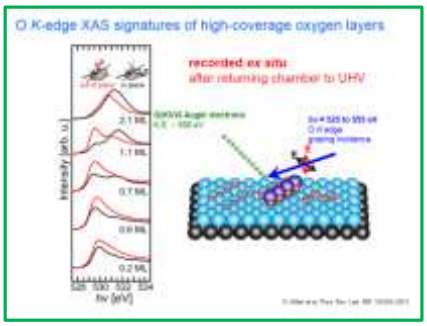
"НА КОКТЕЙЛ ОТ ЗНАНИЯ"

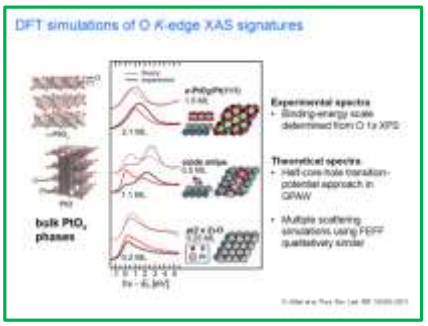


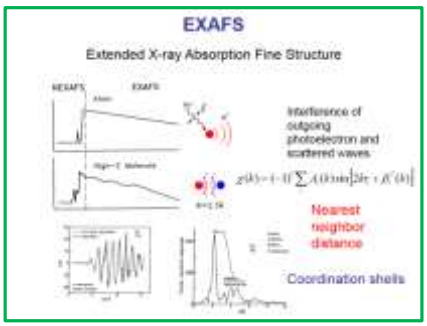


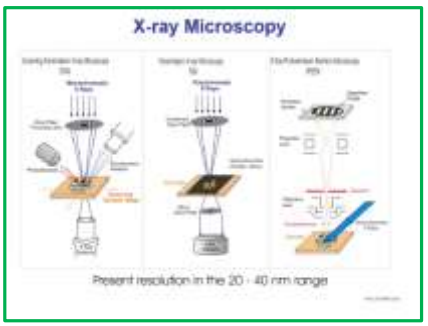












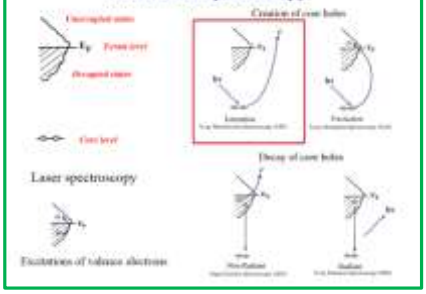
Проект BG05M2OP001-2.009-0028 "Постигане на оптимална среда за обучение, научни изследвания, иновации и устойчиво развитие на човешкия капитал в сферата на химическите науки: Адаптиране на образованието днес за утрешния ден", финансиран от Оперативна програма „Наука и образование за интелигентен растеж“, съфинансирана от Европейския съюз чрез Европейските структурни и инвестиционни фондове.

"НА КОКТЕЙЛ ОТ ЗНАНИЯ"

Theoretical Simulations

- XPS: ΔKohn-Sham
- XAS: Transition potential, TDDFT, CPP
- XES: TDDFT, Kramers-Heisenberg, SC-KH

Core Level Spectroscopy

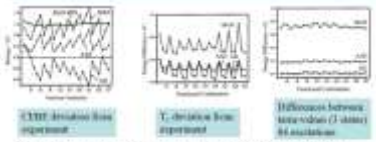


ΔKohn-Sham

- Compute energy difference between ground and core-ionized state
- Equivalent atoms: Select which core-orbital by
  - ➢ removing others using effective core potential
  - ➢ or localizing and freezing
- Shifts more reliable

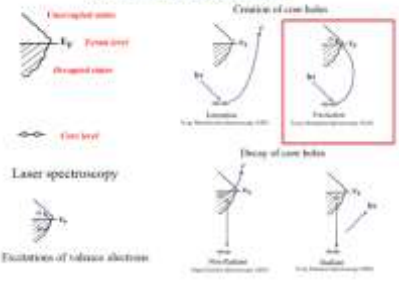
Functional Dependence of XPS and XAS

18 molecules with well-established CEBE and term-values (XAS)
9 exchange functionals x 3 correlation functionals



Most of the error due the functionals are associated with the electron dense inner shell. Cancels for excitation energy differences and XPS shifts. Calibrate against exp. CEBE

Core Level Spectroscopy



X-ray Absorption

Unperturbed Hamiltonian

With E-field — A is the vector potential

Perturbed Hamiltonian

Coulomb gauge

Linearly polarized monochromatic plane wave

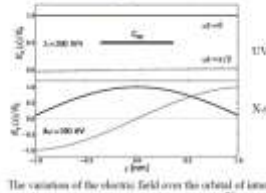
Dipole Approximation

Transition rate

Expand

Write p as the commutator

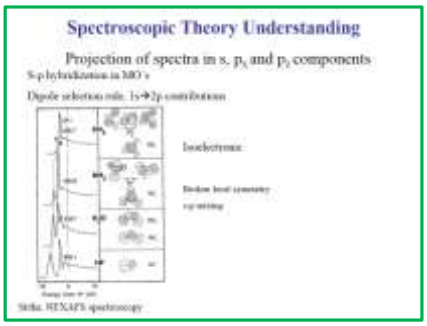
Dipole Approximation

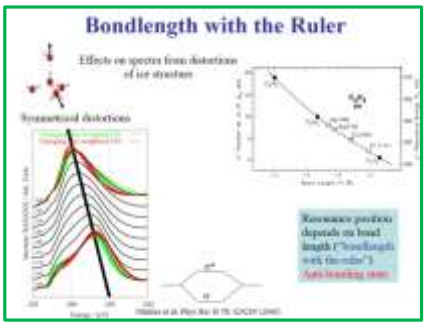


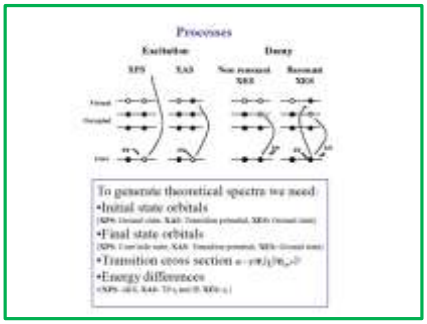
The variation of the electric field over the orbital of interest determines the validity, i.e. $kr \ll 1$ where $k = \frac{2\pi}{\lambda}$

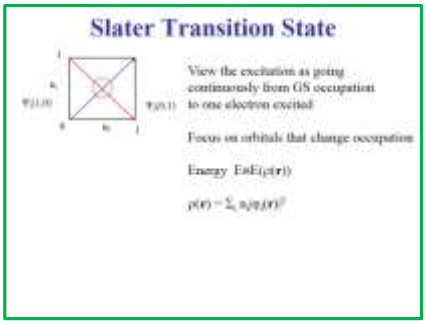
Проект BG05M2OP001-2.009-0028 "Постигане на оптимална среда за обучение, научни изследвания, иновации и устойчиво развитие на човешкия капитал в сферата на химическите науки: Адаптиране на образованието днес за утрешния ден", финансиран от Оперативна програма „Наука и образование за интелигентен растеж“, съфинансирана от Европейския съюз чрез Европейските структурни и инвестиционни фондове.

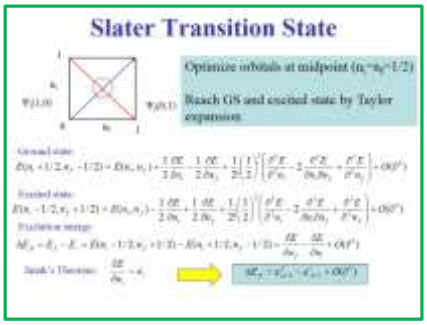
"НА КОКТЕЙЛ ОТ ЗНАНИЯ"

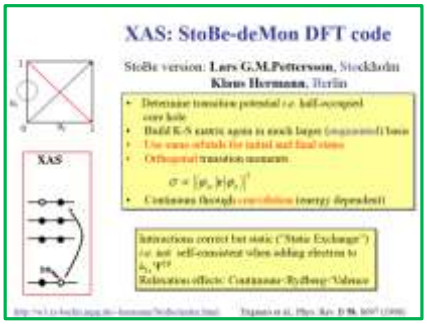






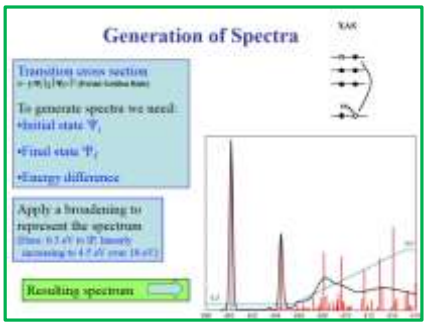


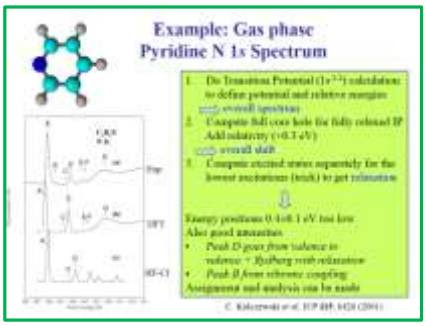


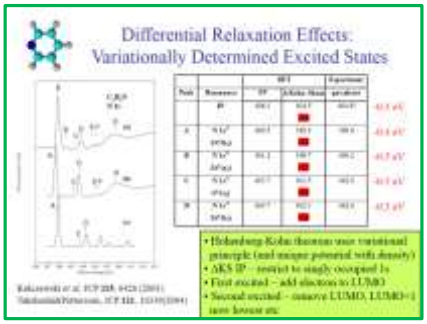


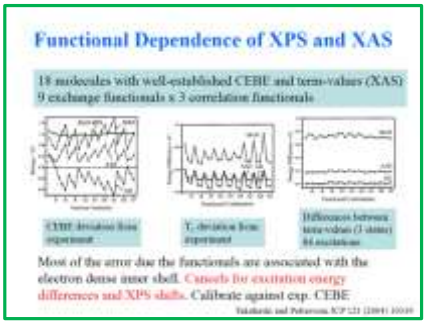
Проект BG05M2OP001-2.009-0028 "Постигане на оптимална среда за обучение, научни изследвания, иновации и устойчиво развитие на човешкия капитал в сферата на химическите науки: Адаптиране на образованието днес за утрешния ден", финансиран от Оперативна програма „Наука и образование за интелигентен растеж“, съфинансирана от Европейския съюз чрез Европейските структурни и инвестиционни фондове.

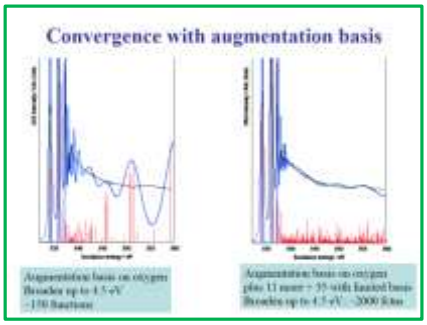
"НА КОКТЕЙЛ ОТ ЗНАНИЯ"

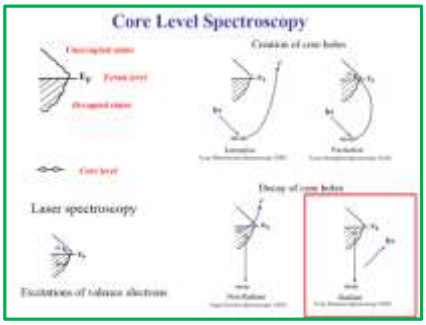


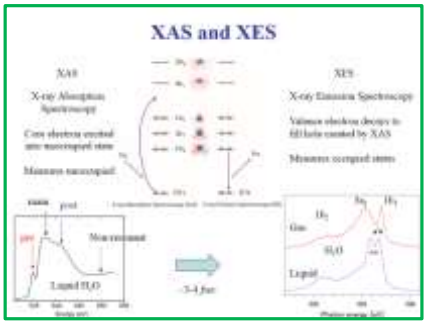


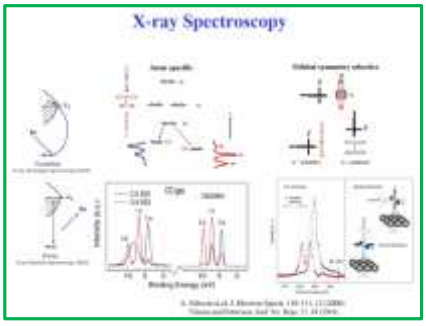






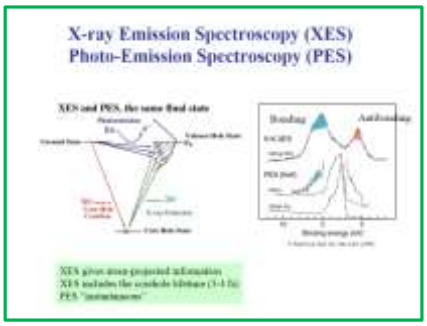


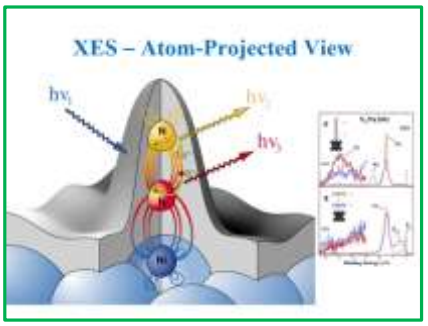


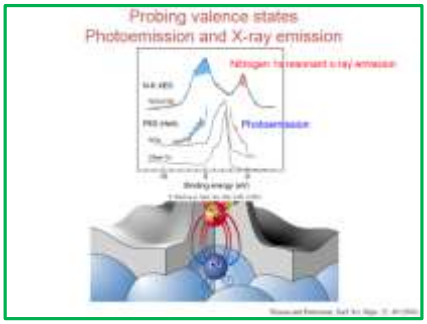


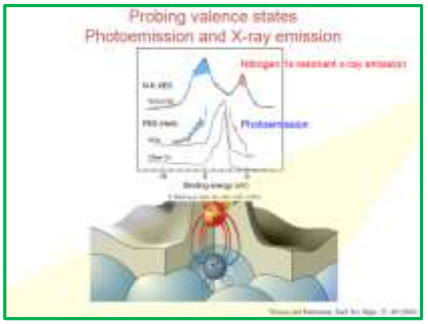
Проект BG05M2OP001-2.009-0028 "Постигане на оптимална среда за обучение, научни изследвания, иновации и устойчиво развитие на човешкия капитал в сферата на химическите науки: Адаптиране на образованието днес за утрешния ден", финансиран от Оперативна програма „Наука и образование за интелигентен растеж“, съфинансирана от Европейския съюз чрез Европейските структурни и инвестиционни фондове.

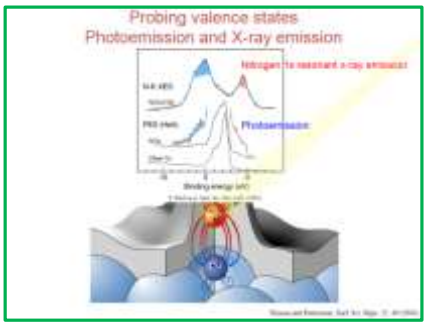
"НА КОКТЕЙЛ ОТ ЗНАНИЯ"

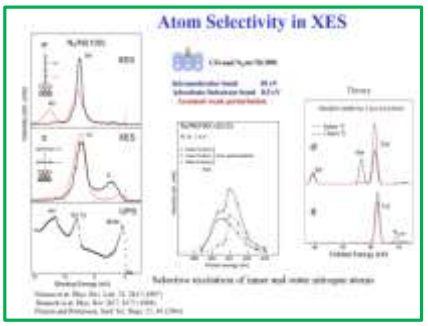


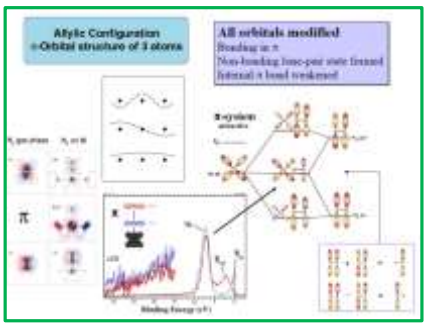


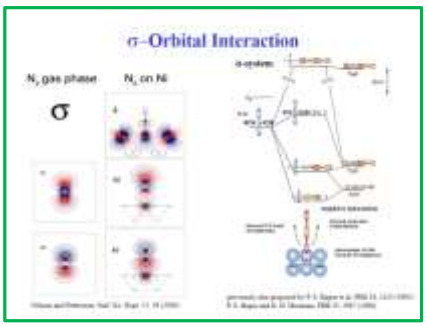






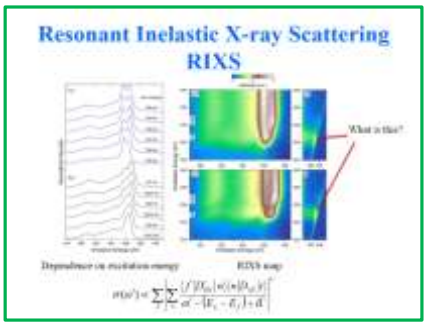


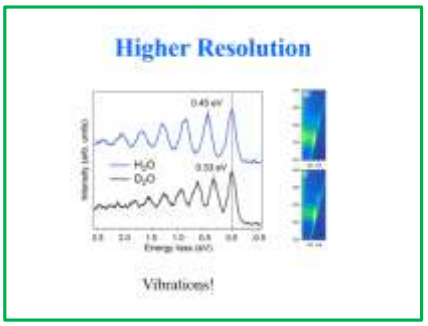


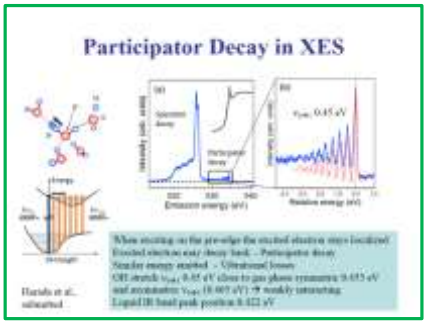


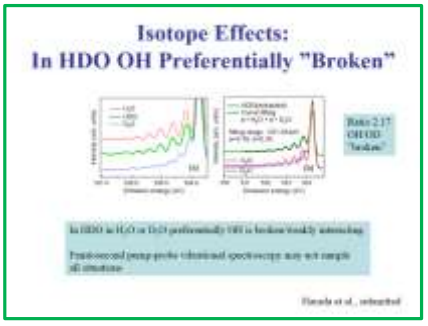
Проект BG05M2OP001-2.009-0028 "Постигане на оптимална среда за обучение, научни изследвания, иновации и устойчиво развитие на човешкия капитал в сферата на химическите науки: Адаптиране на образованието днес за утрешния ден", финансиран от Оперативна програма „Наука и образование за интелигентен растеж“, съфинансирана от Европейския съюз чрез Европейските структурни и инвестиционни фондове.

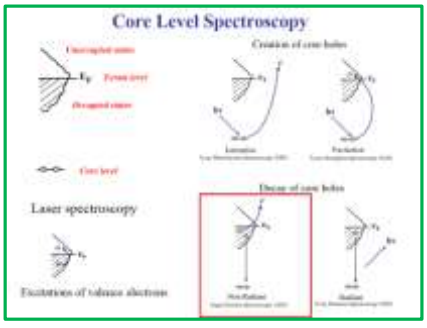
"НА КОКТЕЙЛ ОТ ЗНАНИЯ"

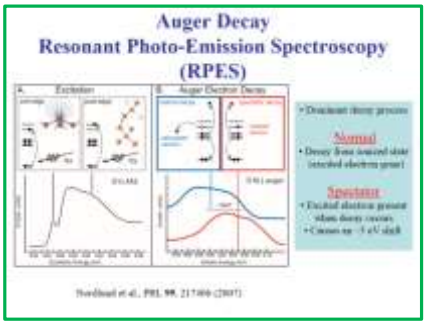


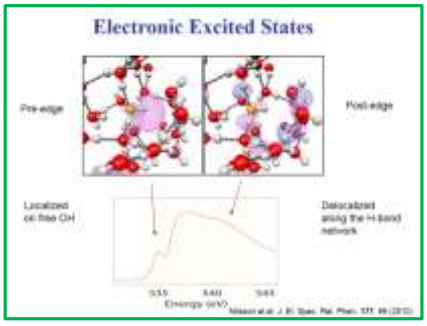


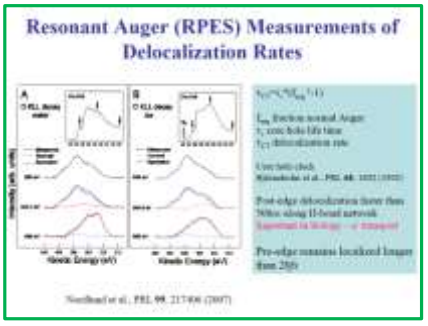






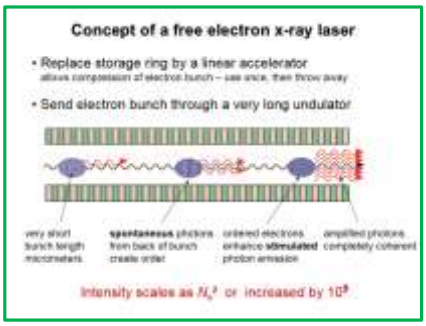


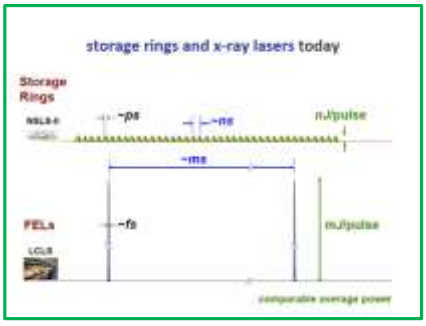


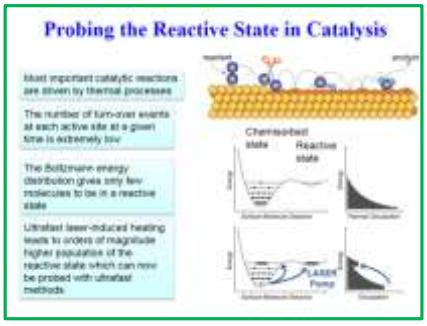


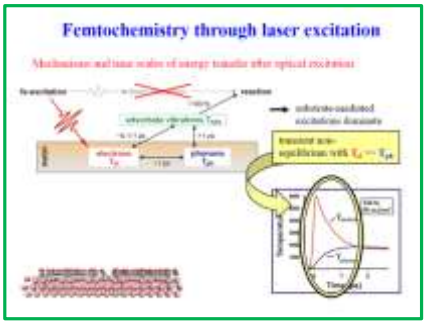
Проект BG05M2OP001-2.009-0028 "Постигане на оптимална среда за обучение, научни изследвания, иновации и устойчиво развитие на човешкия капитал в сферата на химическите науки: Адаптиране на образованието днес за утрешния ден", финансиран от Оперативна програма „Наука и образование за интелигентен растеж“, съфинансирана от Европейския съюз чрез Европейските структурни и инвестиционни фондове.

"НА КОКТЕЙЛ ОТ ЗНАНИЯ"



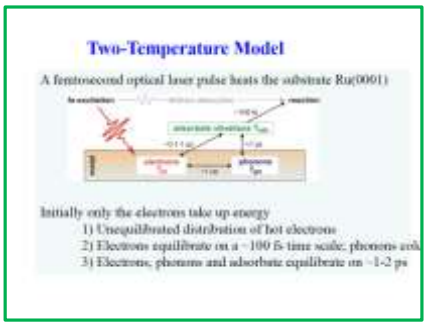


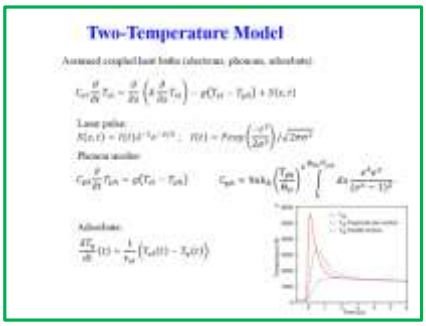


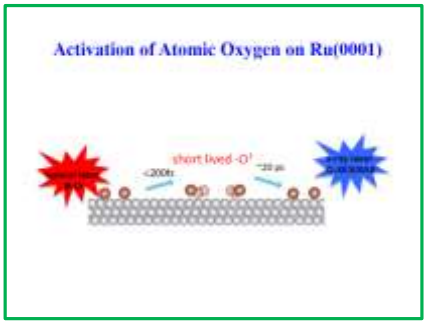


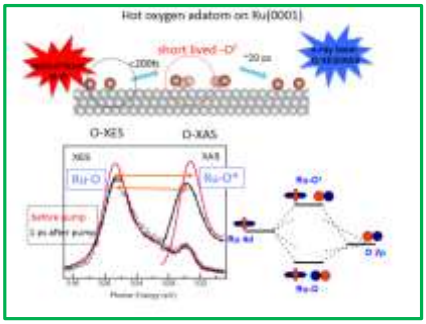
Проект BG05M2OP001-2.009-0028 "Постигане на оптимална среда за обучение, научни изследвания, иновации и устойчиво развитие на човешкия капитал в сферата на химическите науки: Адаптиране на образованието днес за утрешния ден", финансиран от Оперативна програма „Наука и образование за интелигентен растеж“, съфинансирана от Европейския съюз чрез Европейските структурни и инвестиционни фондове.

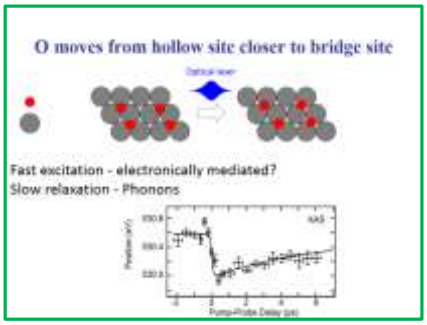
"НА КОКТЕЙЛ ОТ ЗНАНИЯ"

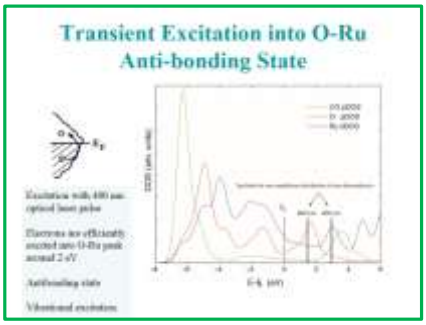


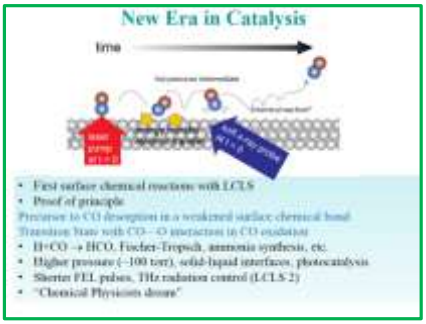












Проект BG05M2OP001-2.009-0028 "Постигане на оптимална среда за обучение, научни изследвания, иновации и устойчиво развитие на човешкия капитал в сферата на химическите науки: Адаптиране на образованието днес за утрешния ден", финансиран от Оперативна програма „Наука и образование за интелигентен растеж“, съфинансирана от Европейския съюз чрез Европейските структурни и инвестиционни фондове.