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First-Principles Simulation of the Absorption Bands of Fluorenone in Zeolite L

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The contents:

1. Test of the value of "N_{config}" (the total number of instantaneous configurations in the sample) used in Equation 2, N_{config} =200, 300, 400, 500, 600, 650.

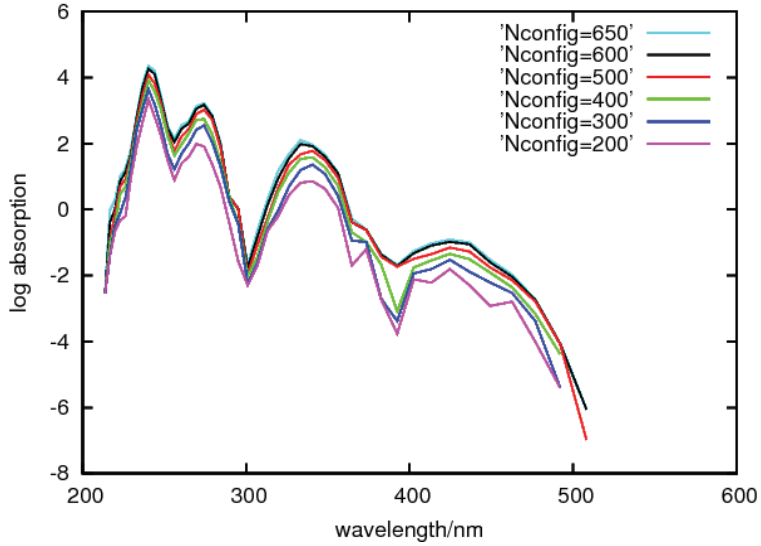

Figure 1. Spectra simulated from different numbers of configurations.

2. Test of the value "*a*" (summation range) used in Equation 2, a = 0.06 eV, 0.08 eV, 0.10 eV, 0.14 eV.

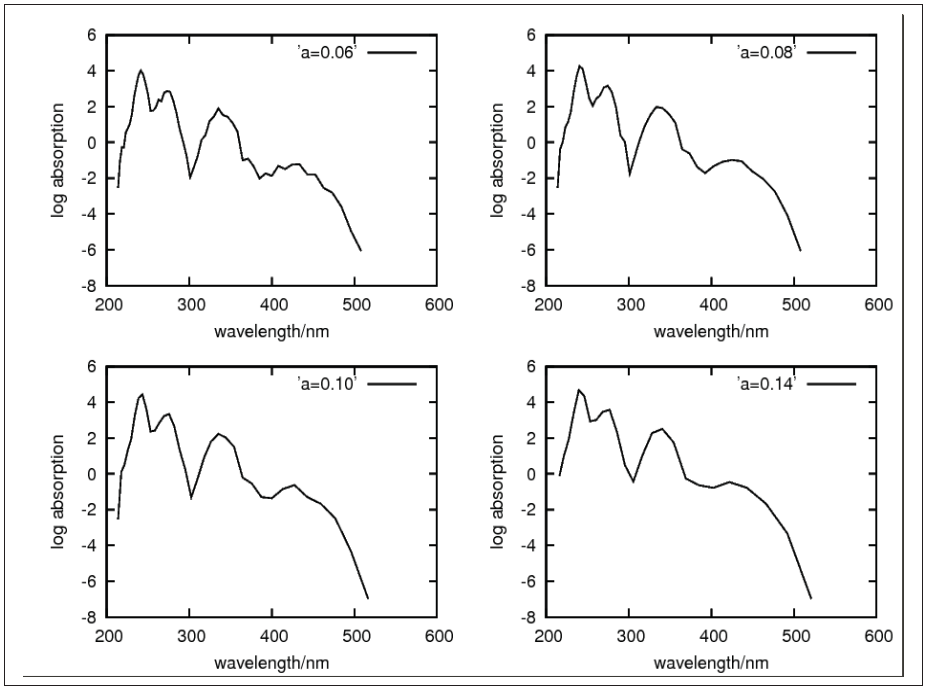

Figure 2. Spectra simulated using different values of the parameter *a* in Equation 2.

3. The effect of the choice of ρ_B in Equation 1 on calculated excitation energies

Model:

Fluorenone: $C_{13}H_8O$ (22 atoms),

Environment: $Si_{50}Al_{16}K_{16}O_{163}H_{62}$ (307 atoms),

Total net charge=0.

The cut bonds are saturated by hydrogen atoms.

The method to generate electron density of

the $Si_{50}Al_{16}K_{16}O_{163}H_{62}$ cluster.

a) ρ_B from Kohn-Sham calculations

b) ρ_B as superposition of spherically symmetric atomic densities

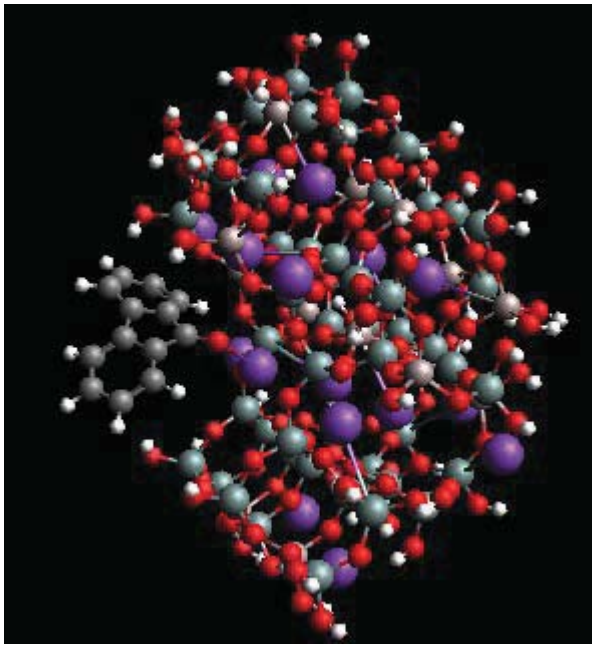

Figure 3. Structure of the cluster $Si_{50}Al_{16}K_{16}O_{163}H_{62}$(Fl)

Excitation energies of fluorenone embedded in the small cluster:

a) ρ_B from Kohn-Sham calculations for the $Si_{50}Al_{16}K_{16}O_{163}H_{62}$ cluster

For each excitation: excitation energies E in a.u. and eV, oscillator strengths f in a.u., dE wrt previous cycle

no.	E/a.u.	E/eV	f	dE/a.u.
1	0.85125E-01	**2.3164**	0.16012E-02	0.54E-08
2	0.11786	3.2072	0.26010E-02	0.32E-08
3	0.12334	3.3562	0.26969E-01	0.17E-07
4	0.13718	3.7328	0.57932E-02	0.25E-07
5	0.15105	4.1102	0.46147E-01	0.46E-07
6	0.16029	4.3616	0.20362	0.22E-07
7	0.16272	4.4279	0.37489	0.23E-07
8	0.16615	4.5211	0.11445E-01	0.26E-07
9	0.17526	4.7690	0.46239E-02	0.45E-06
10	0.17772	4.8361	0.30761E-01	0.20E-06

b) ρ_B as superposition of spherically symmetric atomic densities in the $Si_{50}Al_{16}K_{16}O_{163}H_{62}$ cluster

For each excitation: Excitation energies E in a.u. and eV, oscillator strengths f in a.u., dE wrt previous cycle

no.	E/a.u.	E/eV	f	dE/a.u.
1	0.86309E-01	**2.3486**	0.21357E-02	0.17E-08
2	0.11683	3.1791	0.67695E-02	0.60E-08
3	0.12151	3.3066	0.30147E-01	0.21E-07
4	0.13774	3.7480	0.64472E-02	0.14E-07
5	0.15148	4.1220	0.77947E-01	0.39E-07
6	0.15773	4.2921	0.71092E-01	0.12E-07
7	0.16021	4.3596	0.21680E-01	0.37E-07
8	0.16306	4.4371	0.42017	0.13E-07
9	0.17292	4.7054	0.56213E-02	0.50E-08
10	0.17882	4.8660	0.47209E-01	0.48E-06