
بسم الله الرحمن الرحيم

Relationship between lattice relaxation and electron delocalization in diamond vacancies

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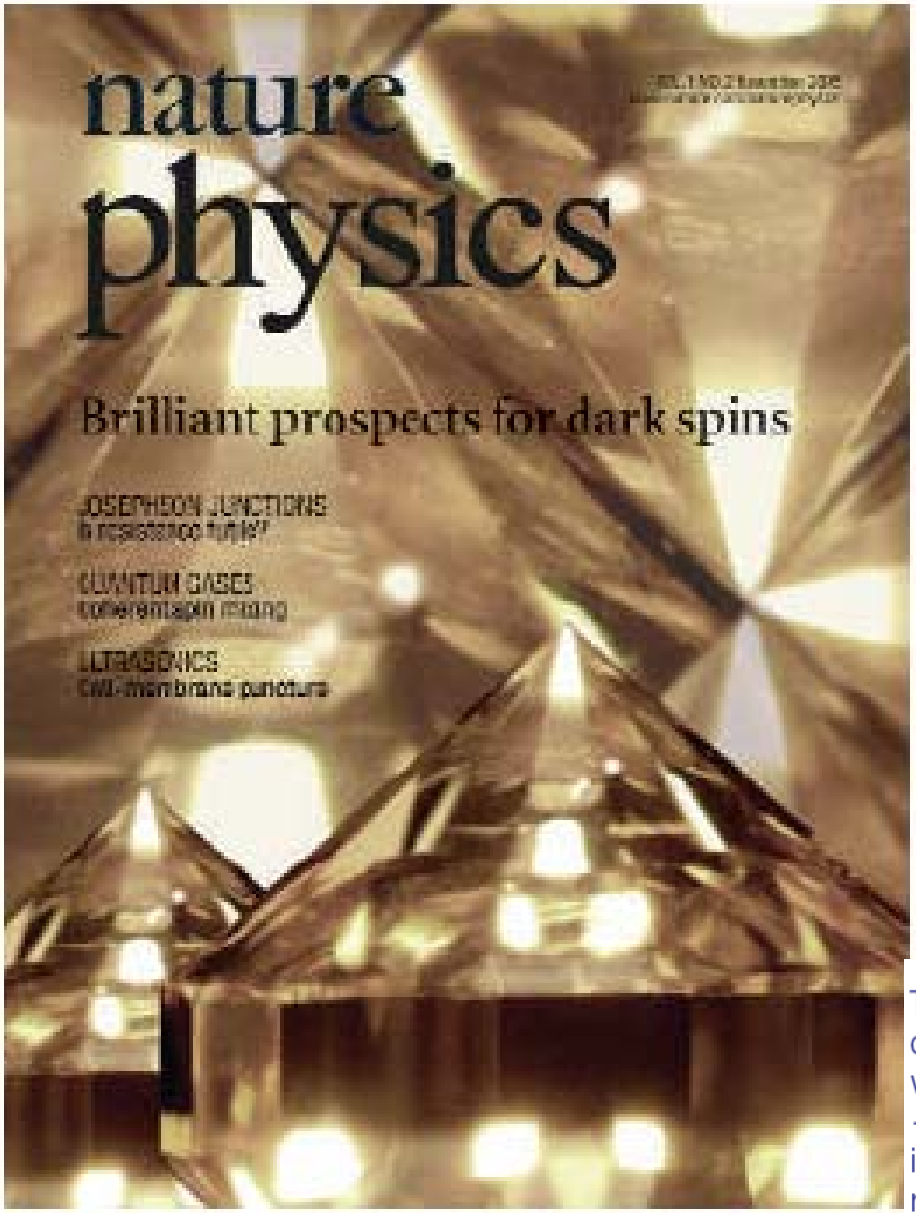
Diamond a promising semiconductor

- High transparency
- Thermal conductivity
- High electron mobility



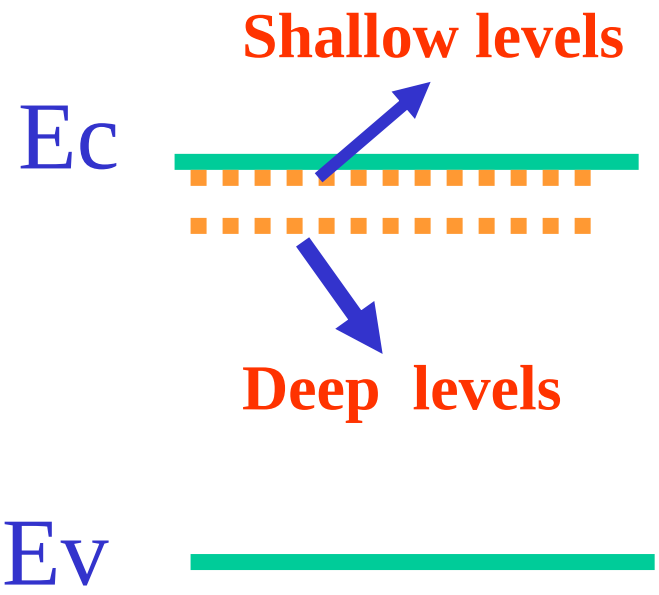
Applications: Spintronics and Solid State quantum information processing

To see a diamond, don't go to a jewellery shop — head for a spintronics or quantum-computation laboratory instead. The spin associated with a nitrogen vacancy centre — an impurity sitting at a vacancy site in the diamond lattice — has a long lifetime and is therefore promising for applications in quantum information processing. Ryan Epstein and colleagues have constructed a room-temperature microscope that is sensitive to the light emitted by a single nitrogen vacancy centre. Moreover, by precisely controlling the magnetic field, they can detect the presence of nearby non-luminescent nitrogen atoms that couple to the nitrogen vacancy centres. These 'dark' spins have an even longer lifetime than the bright spins.

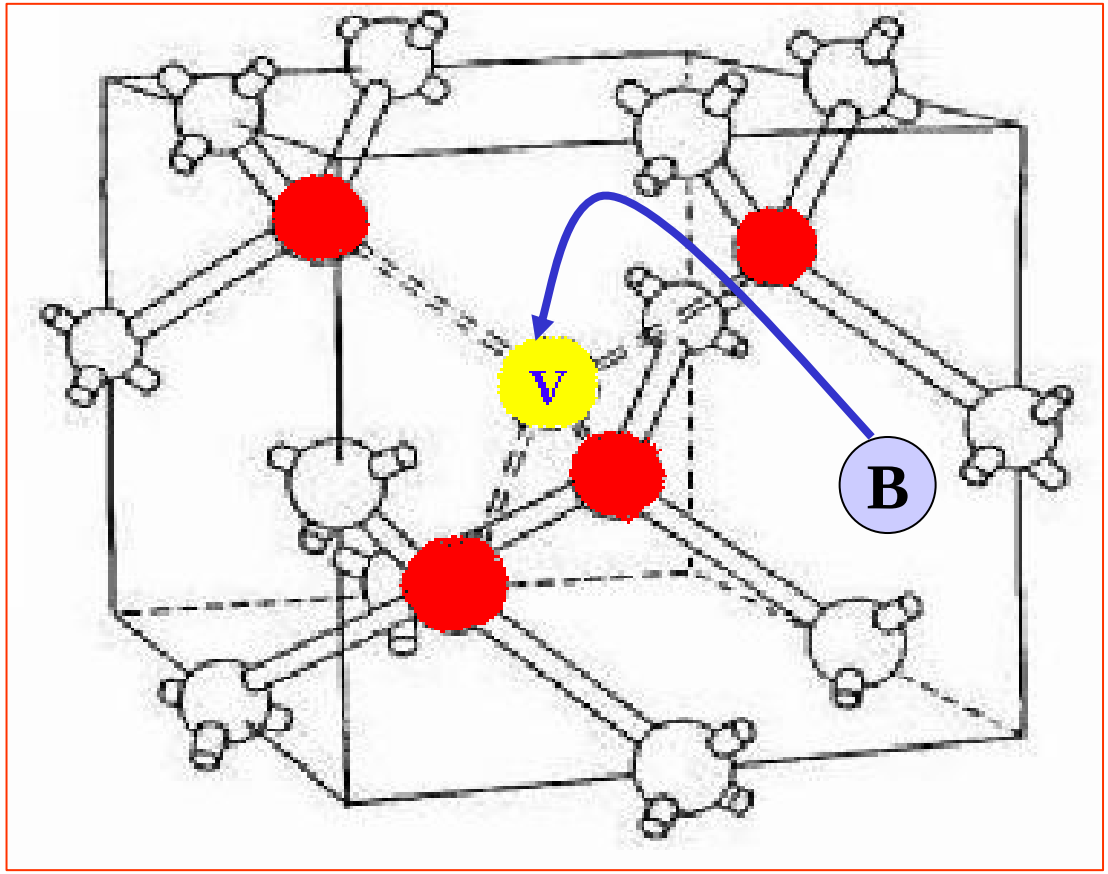
[Letter page 94; News and Views page 79]

Microelectronic Applications

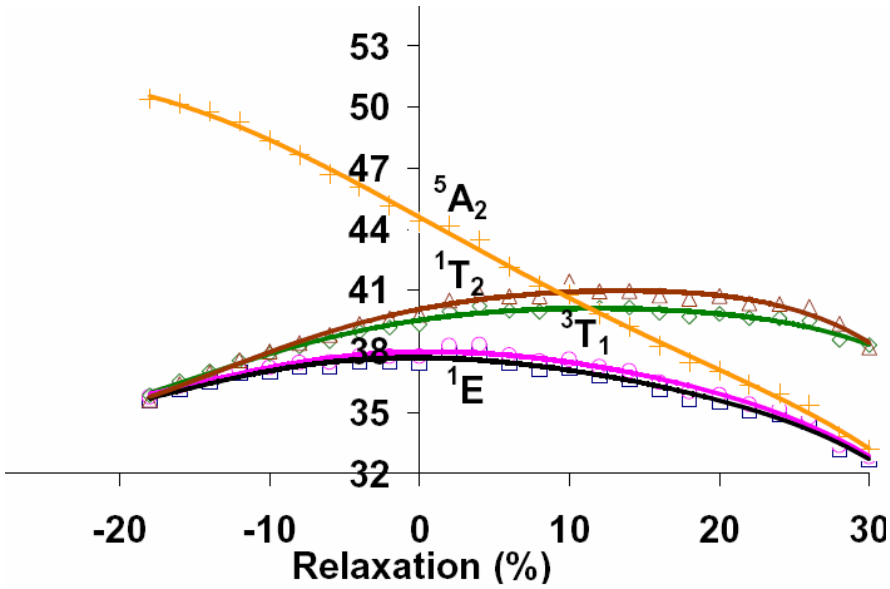
- P-type doping
- N-type doping ???
- Ion implantation
- Thermal diffusions

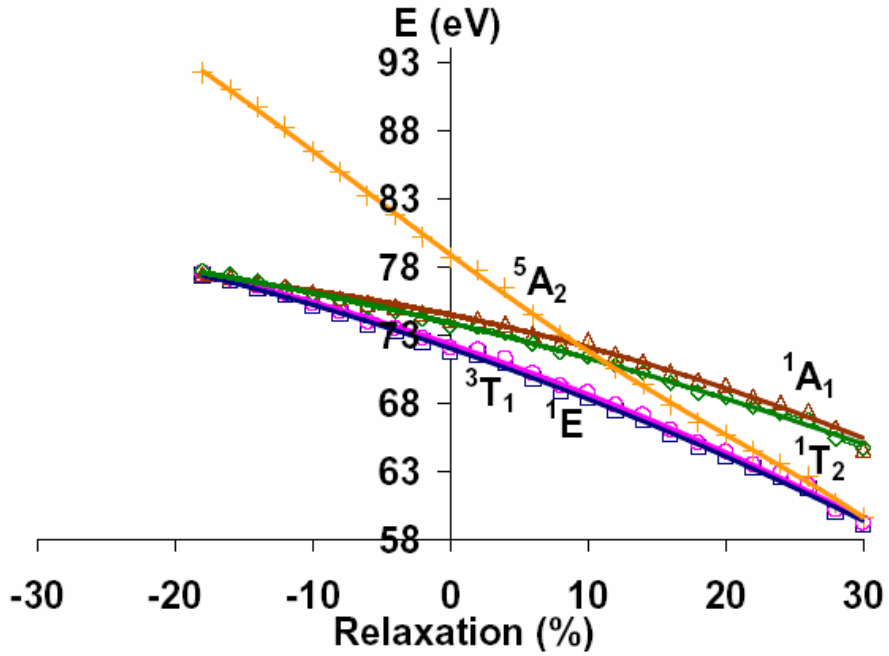


Impurity Substituation Mechanism



Our Previous Work: *Phys. Rev. B*71, 035202 (2005).

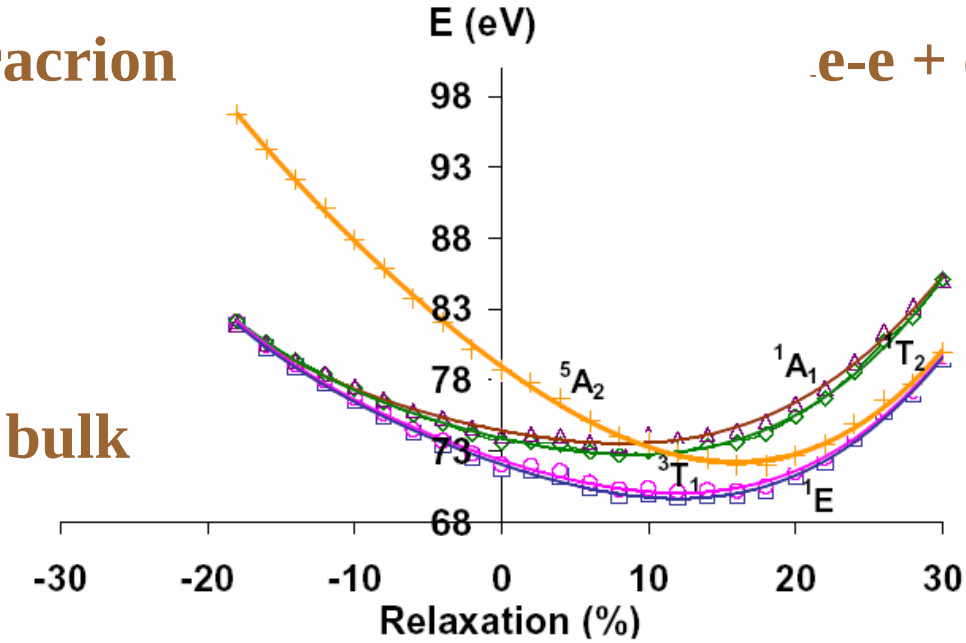




e-e interacrion

e-e + e-i interacrion

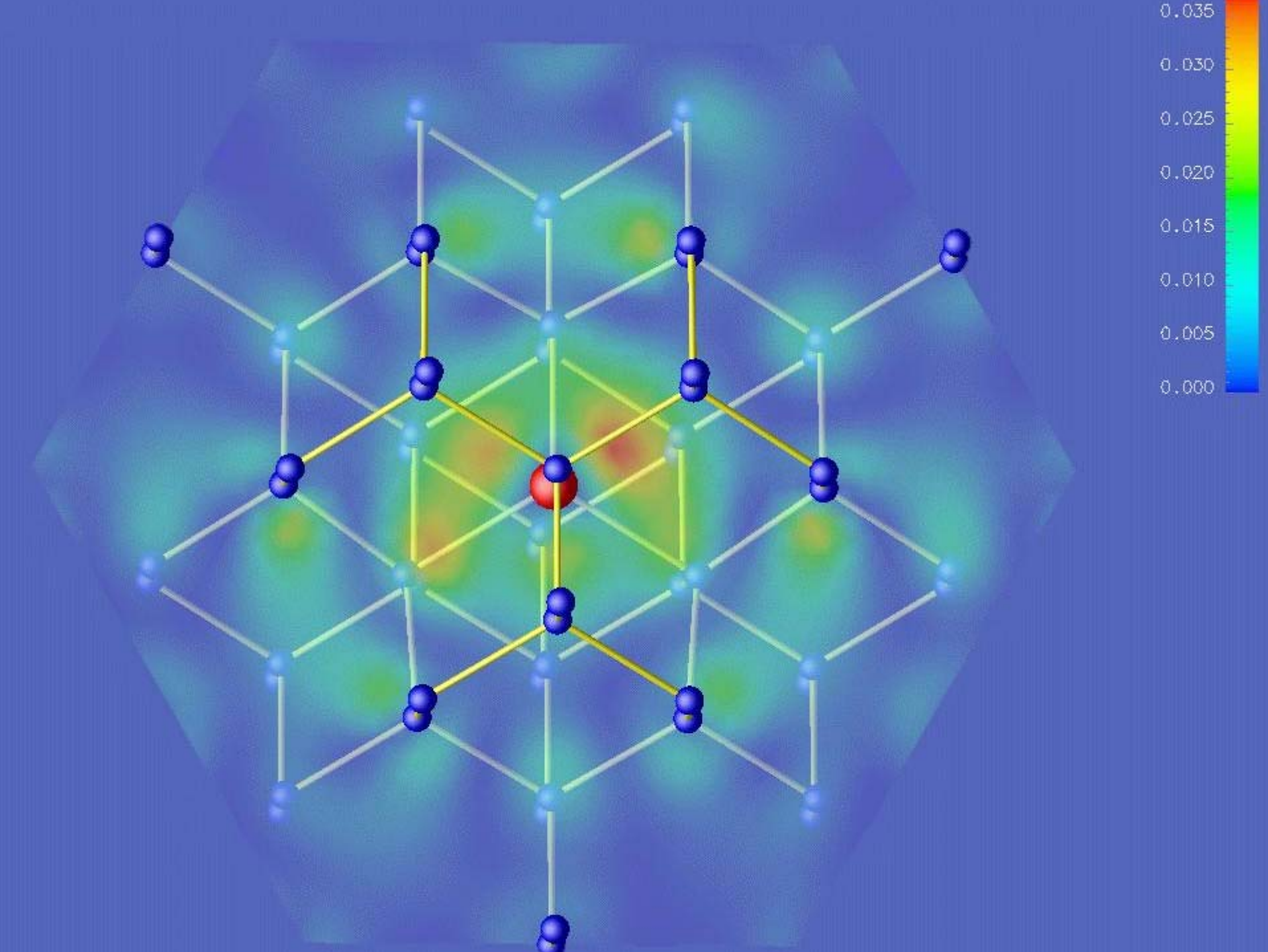
e-e + e-i + elastic bulk interacrion



Microscopic Mechanism behind lattice relaxation

- Electron delocalization
- EPR Experiment
- Ion-ion Screening

M. Heidari Saani et. Al. Physica B 376–377 (2006) 324–326


0.035
0.030
0.025
0.020
0.015
0.010
0.005
0.000

EPR Experiment

- Spin of unpaired electron
- Interaction with B
- Closed shell or singlets
- Free radicals
- Distribution of the unpaired spin density in a molecule
- g-Tensor, Effective spin Hamiltonian

$$\rho_s = \frac{(\rho_\uparrow - \rho_\downarrow)}{N_\uparrow - N_\downarrow}$$

$$H = \beta(B.g.\widetilde{S})$$

EPR Experiment

- EPR Hamiltonian

  Hyperfine splitting (isotope with nonzero nuclear magnetic moment)

$$H = -g_e \beta_e S_z B_z - g_N \beta_N I_z B_z + \sum_{j=1}^{4} S.A^j.I$$

$$\mathbf{A} = a\mathbf{1} + \mathbf{b}$$

- The last term arise from interaction of the unpaired electron and nuclei

$$\Psi = \eta(\alpha\psi_s + \beta\psi_p)$$

EPR Experiment

- Hyperfine parameters

$$a = (2/3)\mu_0 g_e \mu_B g_N \mu_N \eta^2 \alpha^2 |\psi_s(0)|^2$$

$$b = (1/4\pi)\mu_0 g_e \mu_B g_N \mu_N \eta^2 \gamma^2 (\pm 2/5) \langle r^{-3} \rangle_p$$

- Localization

$$\eta^2\alpha^2 + \eta^2\beta^2 = Localization$$

- Relaxation

$$\lambda = \alpha/\beta$$

$$cos^2\theta = (3 + 2\lambda^2)^{-1}$$

Experimental and calculation results

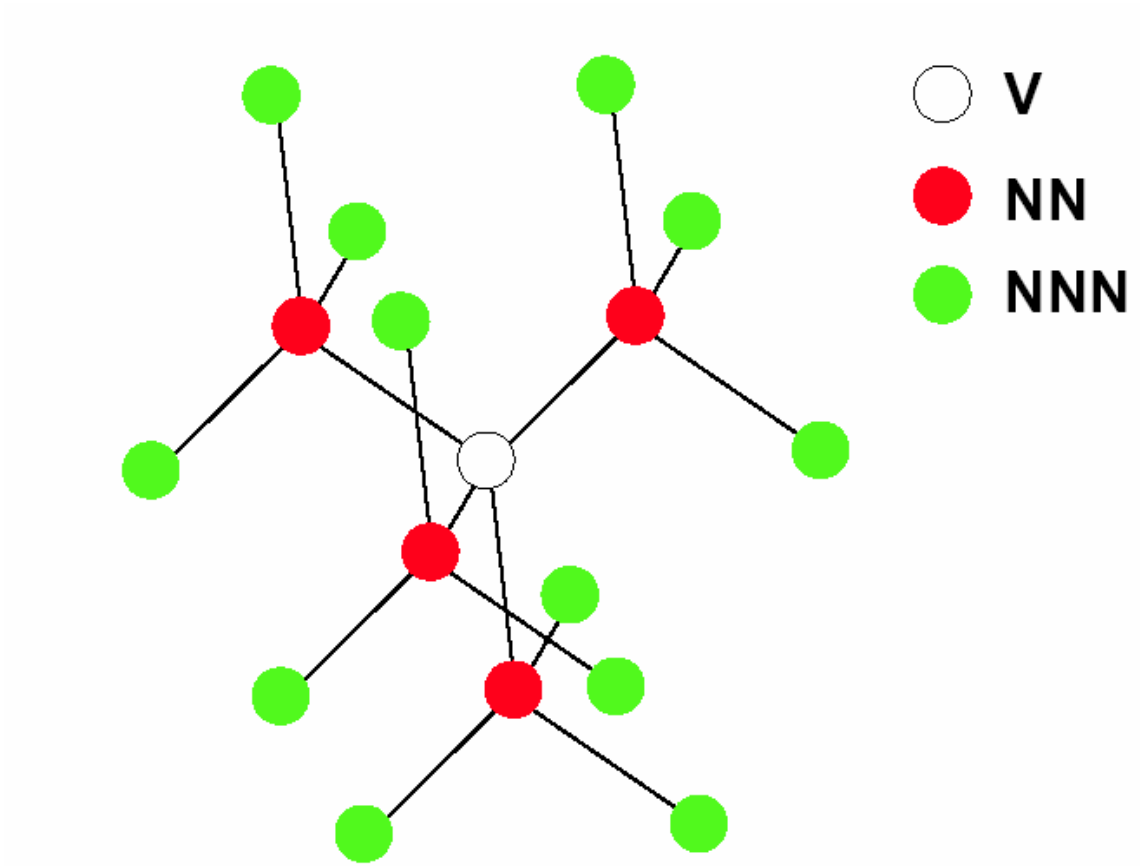
- Recent results (1990's)

	V^0 ($^5A_2$)	V^- (^4A)
Relaxation	15% (18%)	10% (13%)
Lelocalization	75%	85-100%

HFI calculation (DFT) in fair agreement with exp.

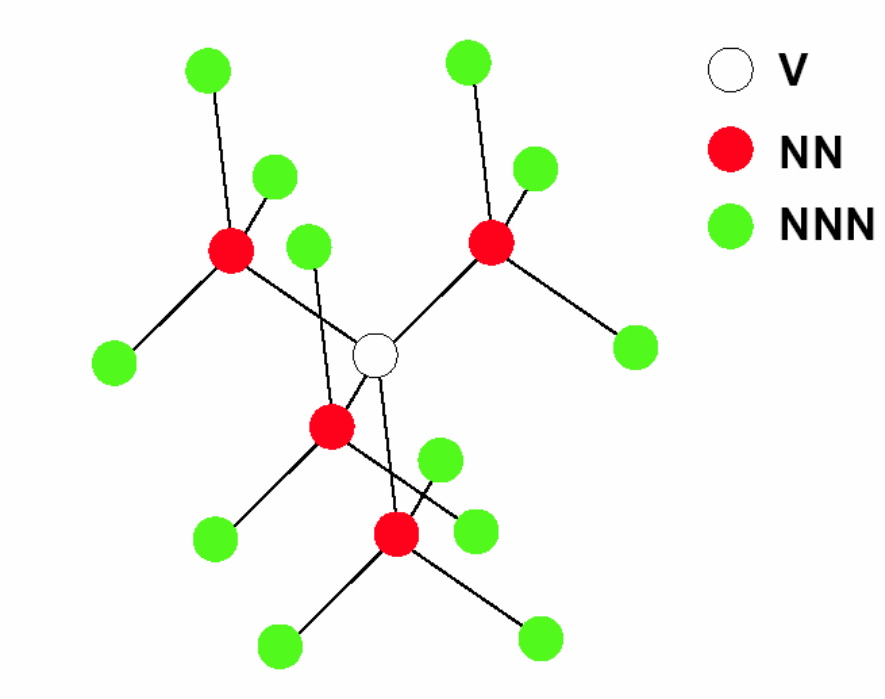
Supercell calculation (Lowther 2001)

- No directional character (s like)
- Order of the charge density on NNN atoms
- Charge density on back bond of NN atoms

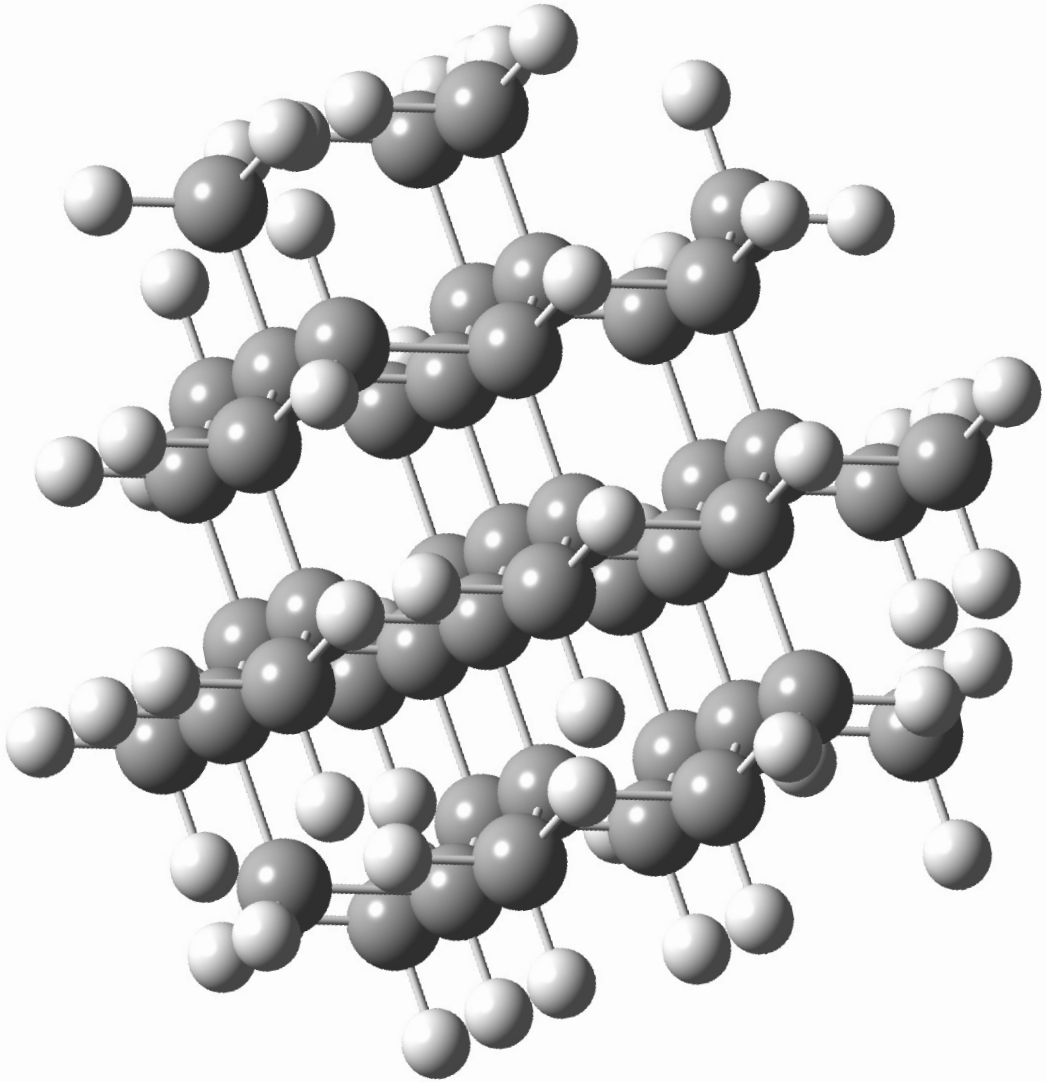


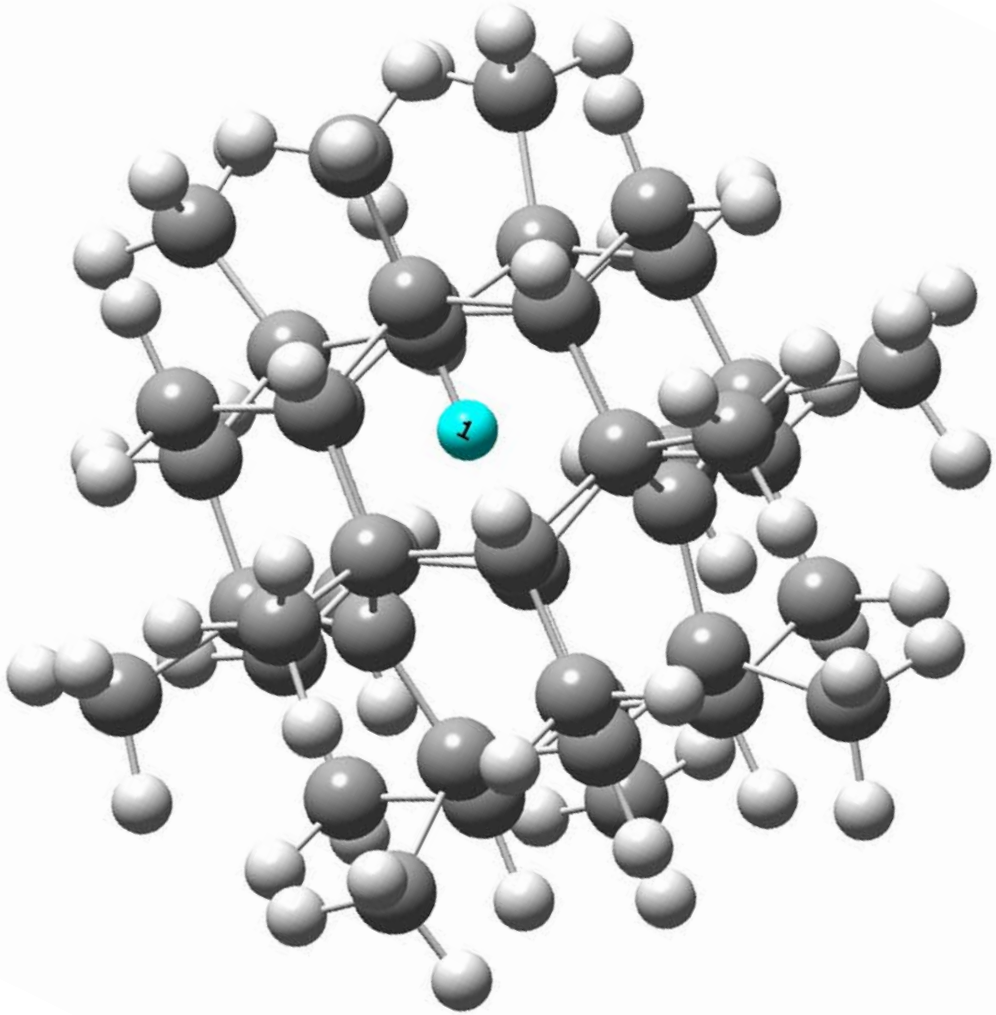
Method:

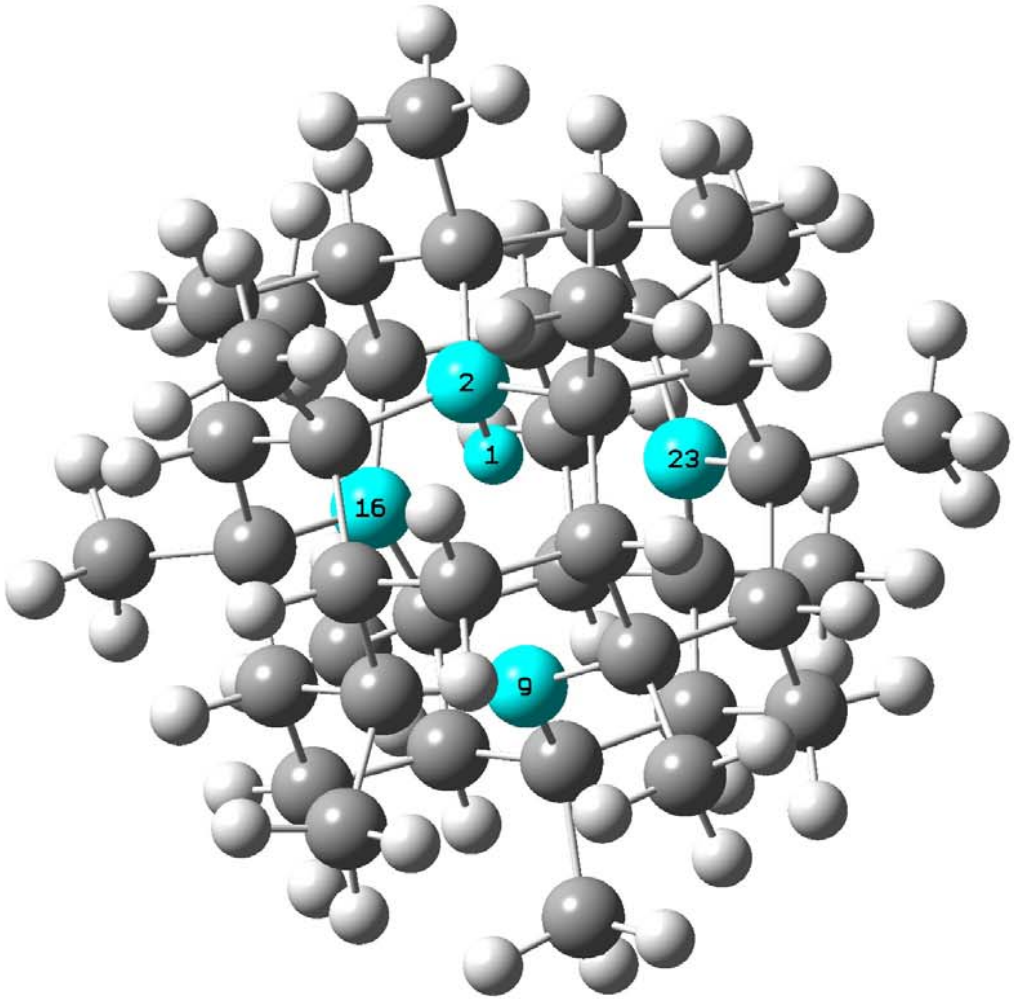
Ab initio Large Cluster DFT ACLCULATION



- Large cluster and hydrogen termination
- Cluster size $C_{93}H_{70}$, $C_{71}H_{84}$ (1995)
- Gaussian basis (6-31G :1s, 2s, 2p,3s, 3p)

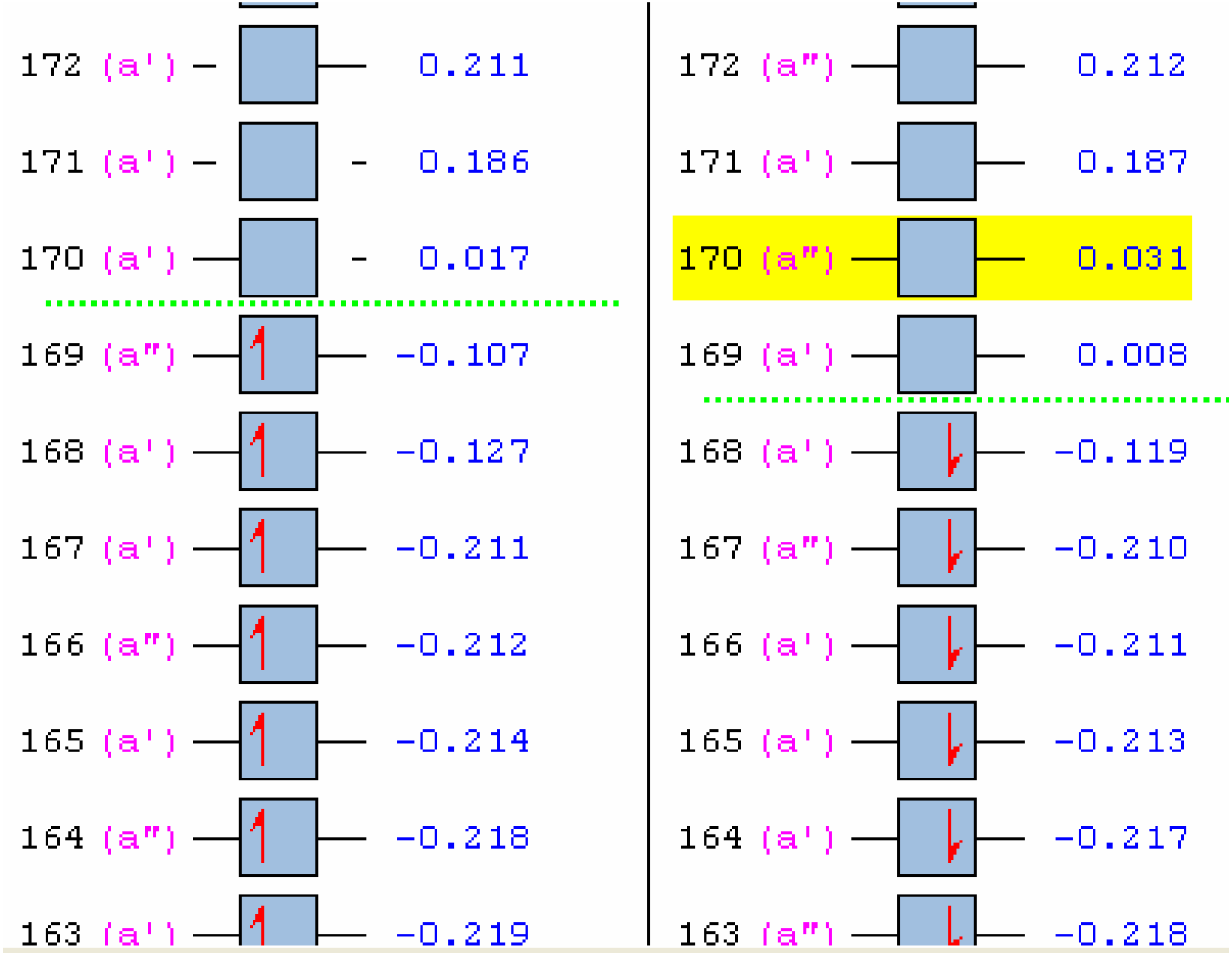



1

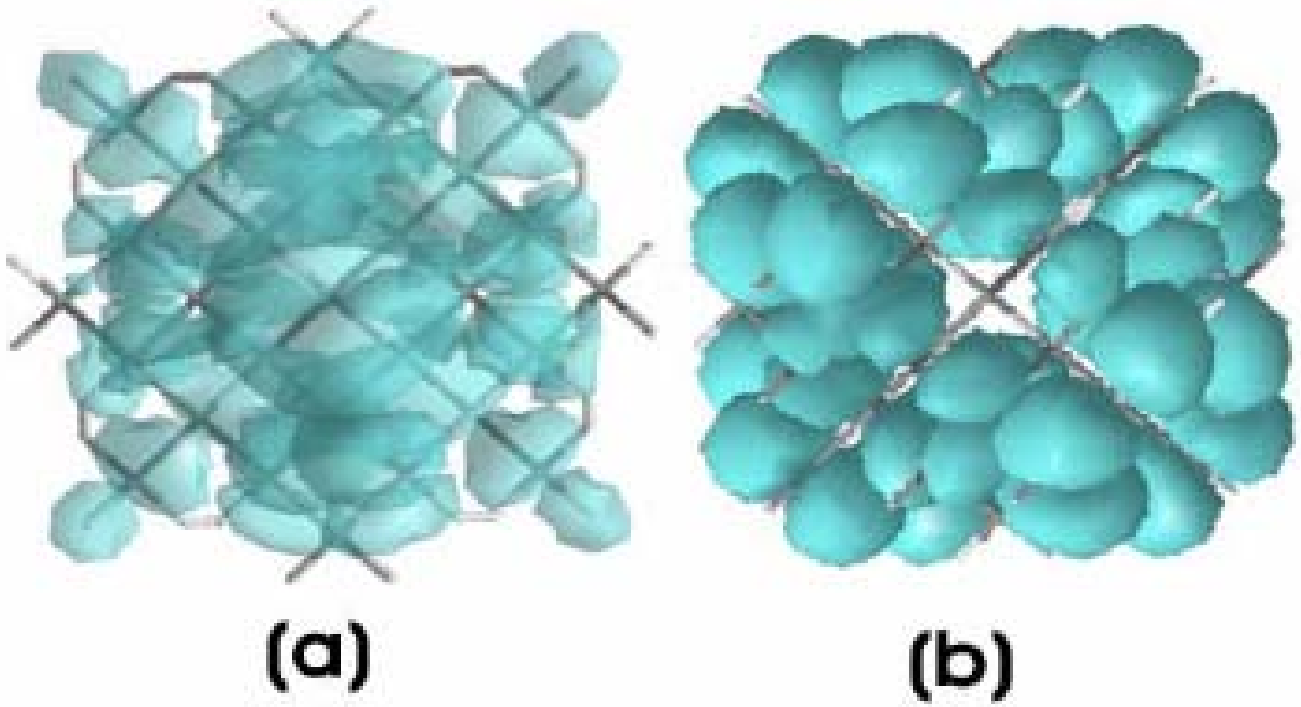

2
1
23
16
9

DFT Calculations

- Comparing Gaussian and plane wave basis
- Innermost basis with 4 exponent and remainder of atoms that have fixed L.C.
- Psedupotential of BHS and All electron calculations
- Ceperely Alder correlation function
- (LDA Or B3LYP)
- Lattice constant and Raman (phonon) frequency
- Relaxation at ground state
- V^0 ($^3T_1$) and V^- ($^4A_2$) :13%


172 (a') 0.211
171 (a') 0.186
170 (a') 0.017
169 (a") -0.107
168 (a') -0.127
167 (a') -0.211
166 (a") -0.212
165 (a') -0.214
164 (a") -0.218
163 (a') -0.219
172 (a") 0.212
171 (a') 0.187
170 (a") 0.031
169 (a') 0.008
168 (a') -0.119
167 (a") -0.210
166 (a') -0.211
165 (a') -0.213
164 (a') -0.217
163 (a") -0.218

C. Effect of delocalization on C-C bondlength



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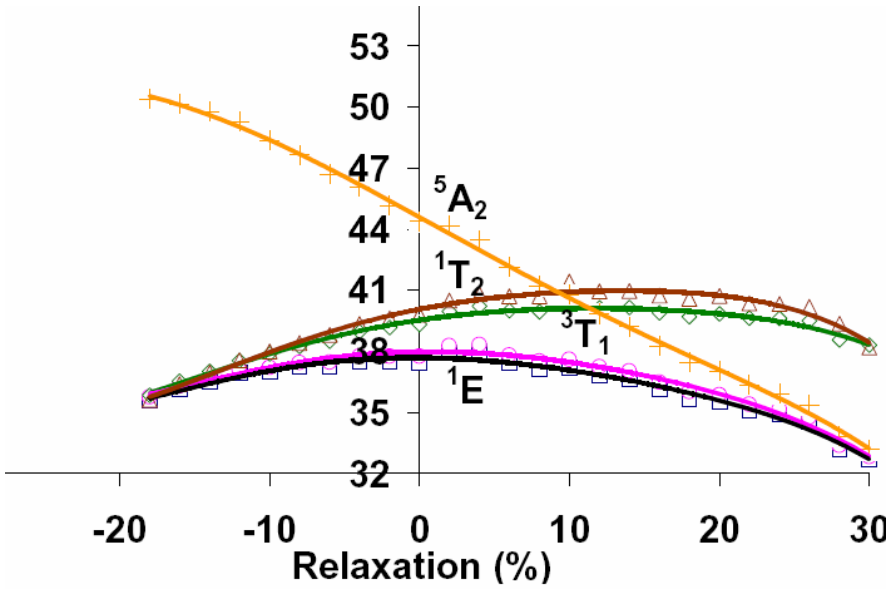
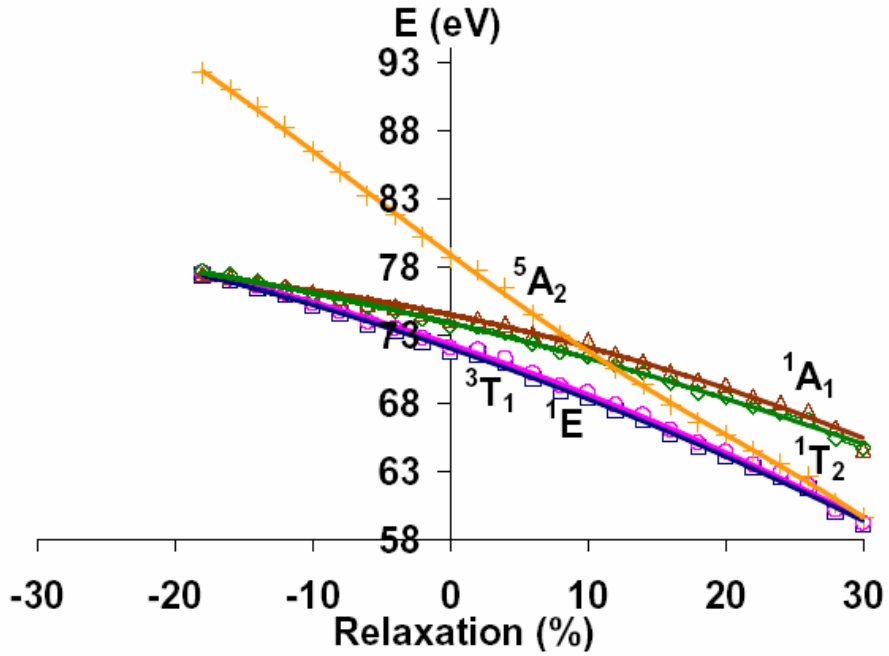
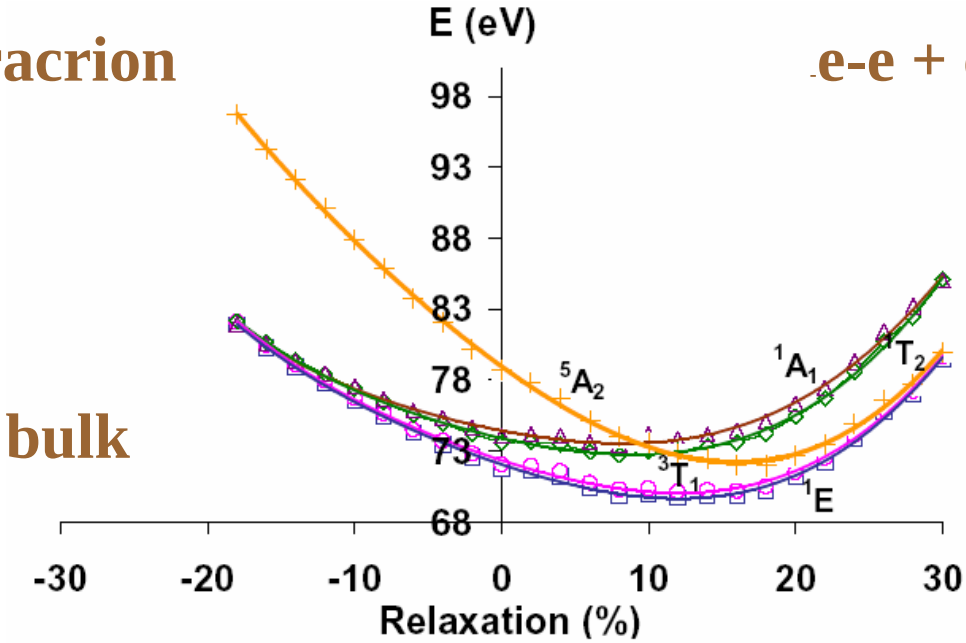


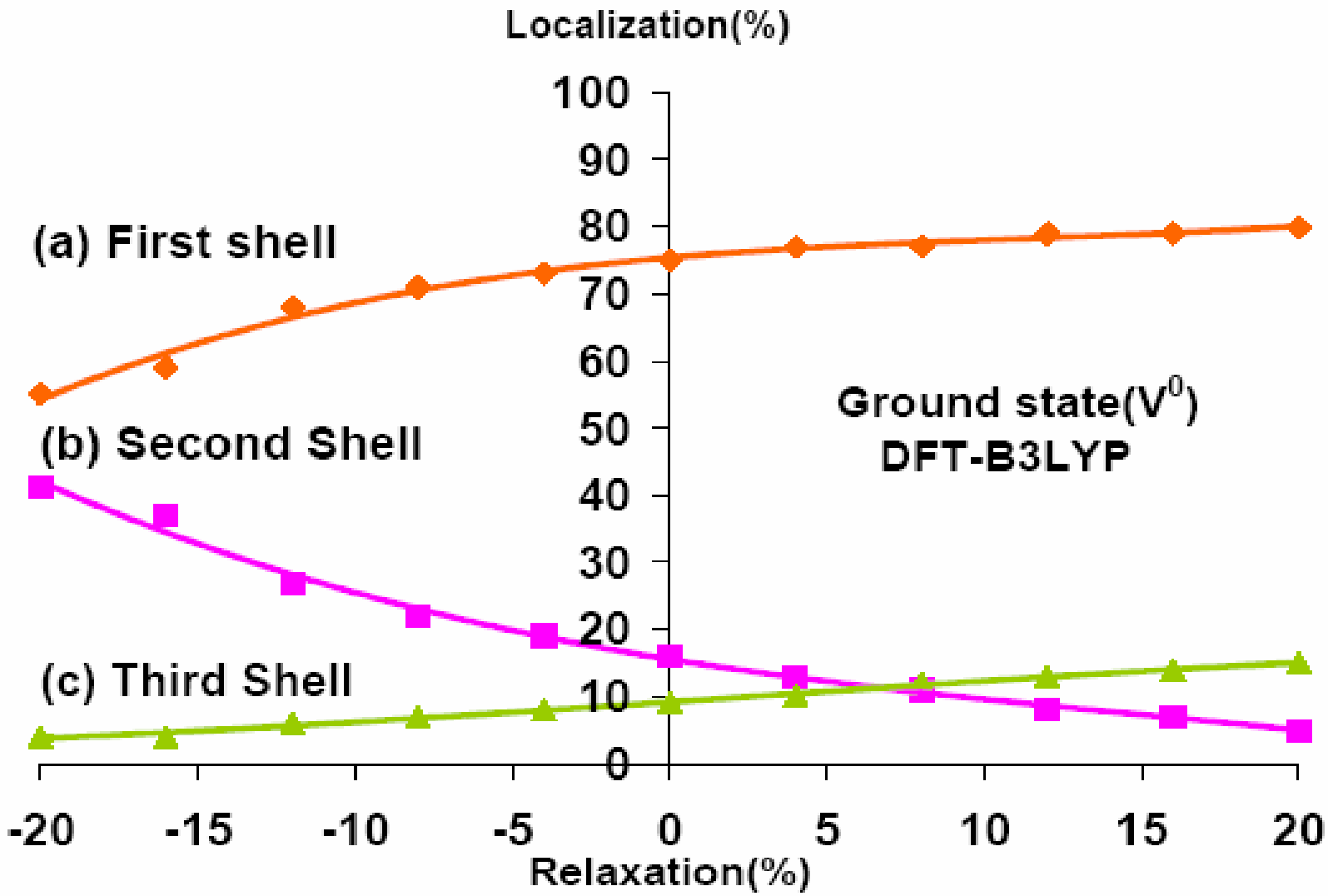


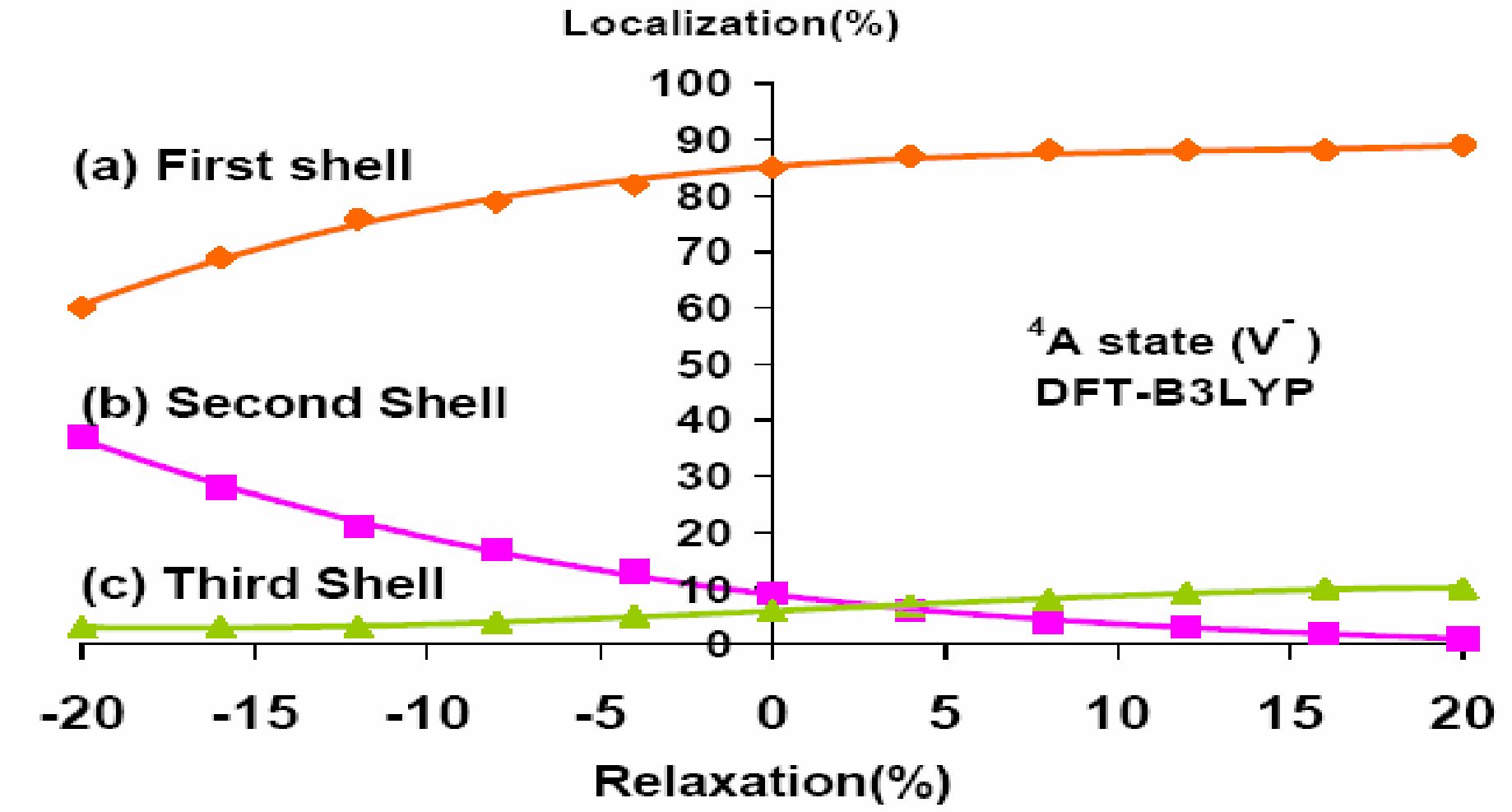
e-e interacrion

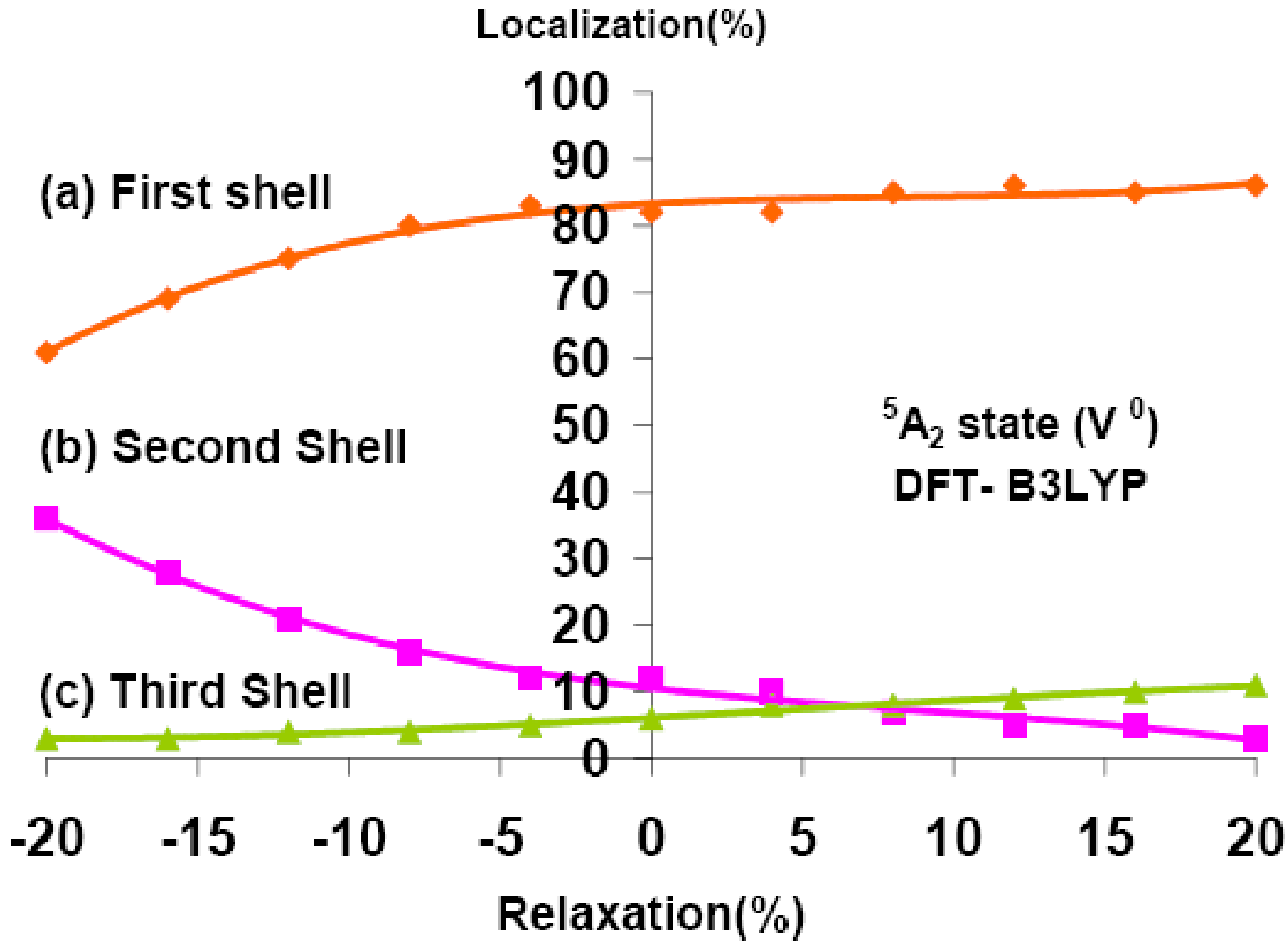
e-e + e-i interacrion

e-e + e-i + elastic bulk interacrion




Localization(%)
100
90
80
70
60
50
40
30
20
10
0
(a) First shell
(b) Second Shell
(c) Third Shell
Ground state(V^0)
DFT-B3LYP
-20
-15
-10
-5
0
5
10
15
20
Relaxation(%)


Localization(%)
100
90
80
70
60
50
40
30
20
10
0
(a) First shell
(b) Second Shell
(c) Third Shell
^{4}A state (V^-)
DFT-B3LYP
-20
-15
-10
-5
0
5
10
15
20
Relaxation(%)


Localization(%)
100
90
80
70
60
50
40
30
20
10
0
(a) First shell
(b) Second Shell
(c) Third Shell
$^5A_2$ state (V^0)
DFT- B3LYP
-20
-15
-10
-5
0
5
10
15
20
Relaxation(%)

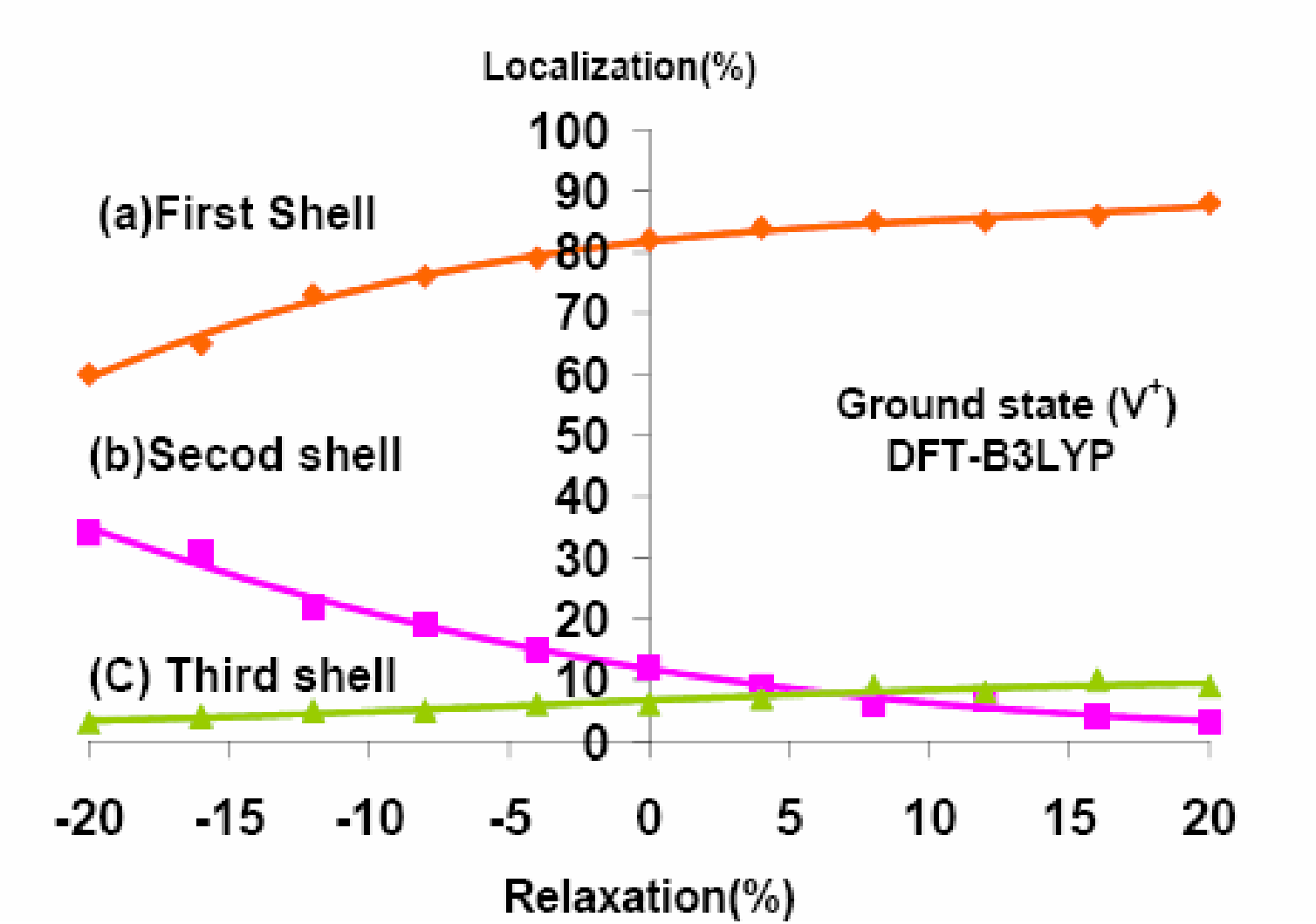
Comparing with EPR on Boron doped diamond

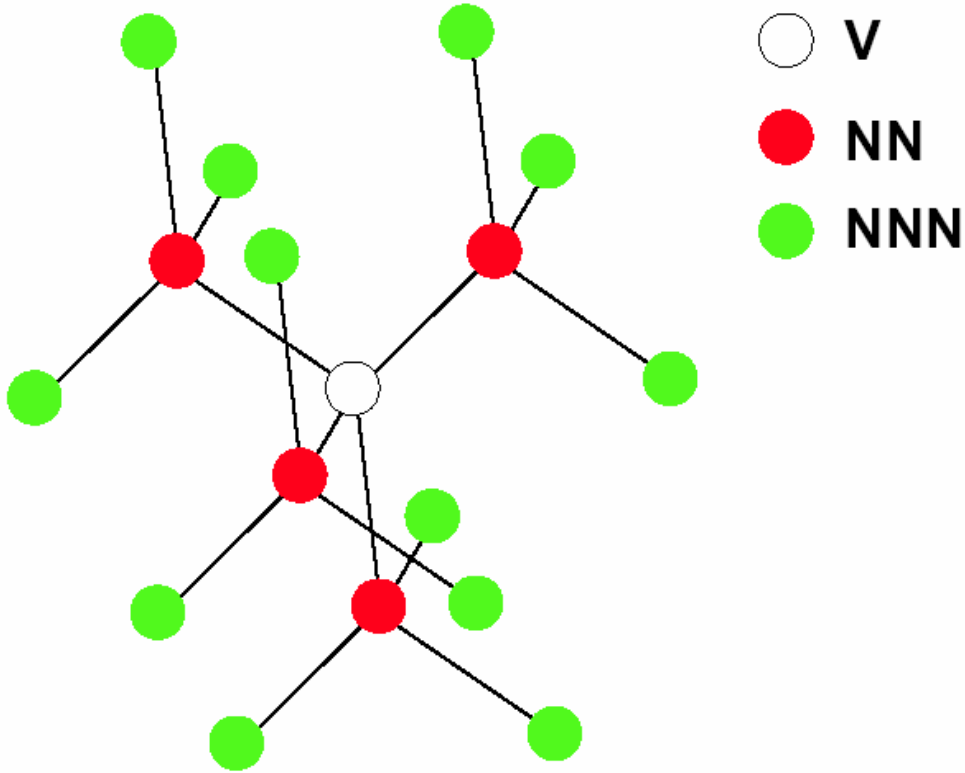
EPR center NIRIM-3 tentatively attributed

$$V^+ \text{ with } S = \frac{1}{2}$$

unpaired spin density on the first neighboring atoms

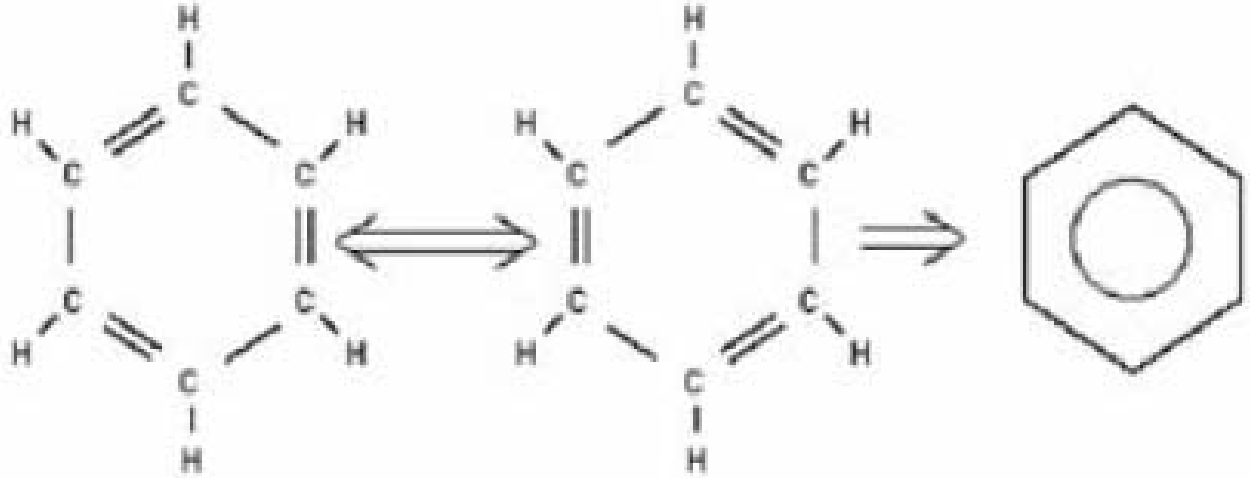
of NIRIM-3 is only 17%.


Localization(%)
100
90
80
70
60
50
40
30
20
10
0
(a)First Shell
(b)Secod shell
(C) Third shell
Ground state (V^+)
DFT-B3LYP
-20
-15
-10
-5
0
5
10
15
20
Relaxation(%)



Charge States	V^0	V^0	$V-$	$V+$
Spin	0	2	3/2	1/2
Electron Density (%)	38	36	43	45

(a)



D. Limitation of semiempirical potentials

Conclusion:

A. Comparison with EPR measurement results

B. Effect of NN ion screening

C. Effect of delocalization on C-C bondlength

D. Limitation of semiempirical potentials

M. Heidari Saani et. Al. Submitted to PRB (2006)