Non-metallic systems – Muonium spectroscopy

Steve Cox

Mu$^+$ (100G)  
Atomic muonium, Mu$^0$  
$A_0 = 4.5 \text{GHz} = 100\%$

1973: Brewer et al

Quartz

1S$_{1/2}$  
2S$_{1/2}$

2P$_{1/2}$

2P$_{3/2}$

Huh?...

Quasiatomic: 50%

Energy levels for vacuum-state muonium.
Hyperfine constants: assignments and systematics

Si$_{0.8}$Ge$_{0.2}$ (King et al, 2005)

Normalized Hyperfine Constant $A/A_0$ (Mu)

Bandgap (eV)

As Si Ge P I GaAs GaP SiC ZnSe ZnS c-BN Diamond NaI RbI KI AlN RbBr KBr KCl NaCl SiO$_2$ NaF LiF MgO InSb Xe Kr Ar

Quasi-atomic

Atomic

100%

1s(H) or 1s(Mu)

50-100%

Fourier Power (arb. units)

Frequency (MHz)

μ$_{34}$ (BC)

ν$_{12}$ (BC)

μ$_{12}$ (T)

ν$_{12}$ (H)

ν$_{34}$ (BC)

ν$_{34}$ (Mu+)

1350 1400 1450

Si$_{0.8}$Ge$_{0.2}$ (King et al, 2005)
Metastability in Si, GaAs etc: cage-centre versus bond-centre

![Molecular orbital model for Mu$_{BC}$ (Cox and Symons '86)](image)

Simulation (Ewels)

Interplay of site and charge state

Electrical activity

- Conduction band
- Valence band

<table>
<thead>
<tr>
<th>Charge State</th>
<th>Donor Depth</th>
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<tbody>
<tr>
<td>$\text{Mu}^0$</td>
<td>210 meV ($\text{Mu}_{BC}^{0/+}$)</td>
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<tr>
<td>$\text{Mu}^+$</td>
<td>175 meV ($\text{H}_{BC}^{0/+}$)</td>
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</table>
Electrical activity: capture, loss and scattering of carriers

Charge exchange

Spin exchange
Conduction band

\[ \text{Valence band} \]

\[ E_F \]
Donor, acceptor and pinning levels

(a) Silicon

(b) Diamond

Van de Walle et al, 1998

Wang and Zunger, 2002
Shallow-donor states

(a) 

Muon decay asymmetry vs. Time (microseconds) for CdS (Gil et al, 1999).

(b) 

Spectral Power (a.u.) vs. Frequency (MHz) for shallow-donor states.

(c) 

Asymmetry (%) vs. Frequency (MHz) for CdS at different temperatures.

(d) 

Energy levels of muons in conduction and valence bands with a 26meV gap, E_D = 26meV.
Almost all muonia!  (Well, except all the organic radicals....)
The deep-to-shallow instability
The deep-to-shallow instability

[Graph showing the relationship between electron affinity (eV) and normalized hyperfine constant $A/A_0$.]
The deep-to-shallow instability
The deep-to-shallow instability

![Graph showing normalized hyperfine constant vs electron affinity for various materials including SiO$_2$, MgO, C (diamond), AlN, ZnS, ZnSe, GaP, GaAs, SiC, Ge, Si, InSb, and $H^0$.](image)
The deep-to-shallow instability
The deep-to-shallow instability

\[ \text{H}^0 \rightarrow \text{H}^+ + e_c \]
The deep-to-shallow instability

$H^0 + O^{2-} \rightarrow OH^- + e_c$

Other oxides and high-k dielectrics

+ other new electronic materials...