UNIVERSITÀ DEGLI STUDI DI TORINO

Point Defects in Diamond: Raman Features of the Isolated **Neutral Vacancy**

Simone Salustro

To infinity and beyond

- All *ab-initio* calculations have been performed with

a computational tool for solid state chemistry and physics

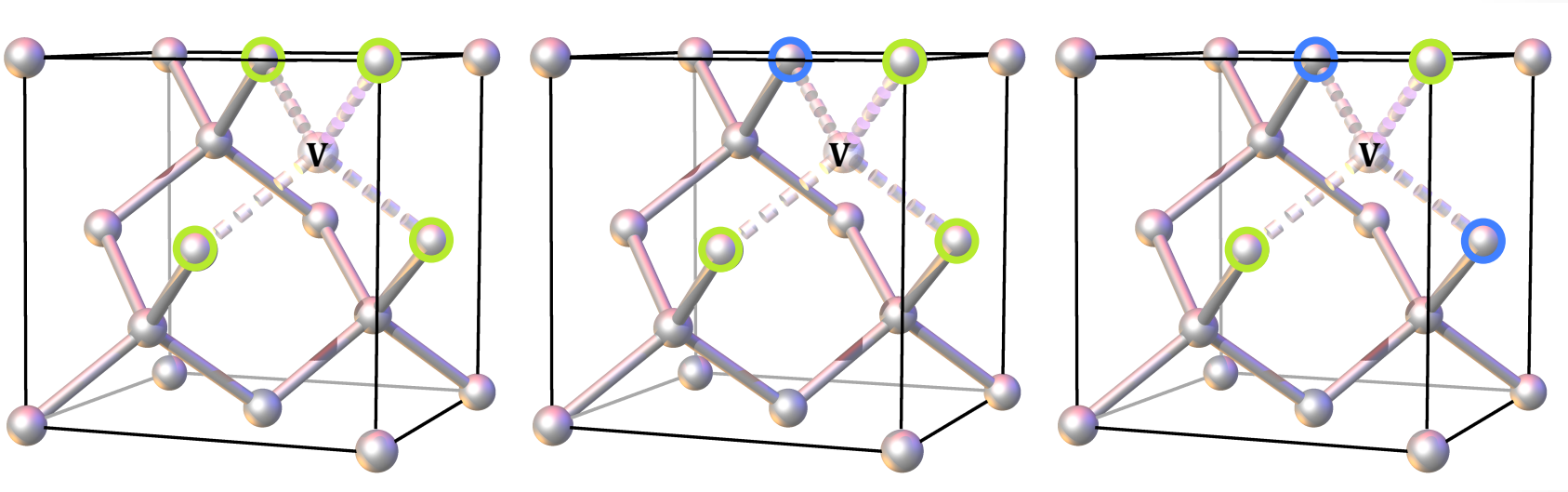
CRYSTAL[1]

- Calculations on 0D, 1D, 2D and 3D periodic systems
- Full exploitation of the symmetry
- Gaussian *all-electron* basis functions
- HF and DFT (Local, GGA, M-GGA, Hybrids, Double Hybrids, LC-)
- EOS, Thermal Expansion, Analitycal Hyperpolarizabilities…
- **++ Frequency calculation & IR/RAMAN intensities ++**

[1]Dovesi *et al.*, *Int J. Quantum Chem.*, **114**:1287, 2014

The Isolated Vacancy

- Single determinant approach.
- Unit cells with 31, 63 and 127 atoms. Different concentrations!



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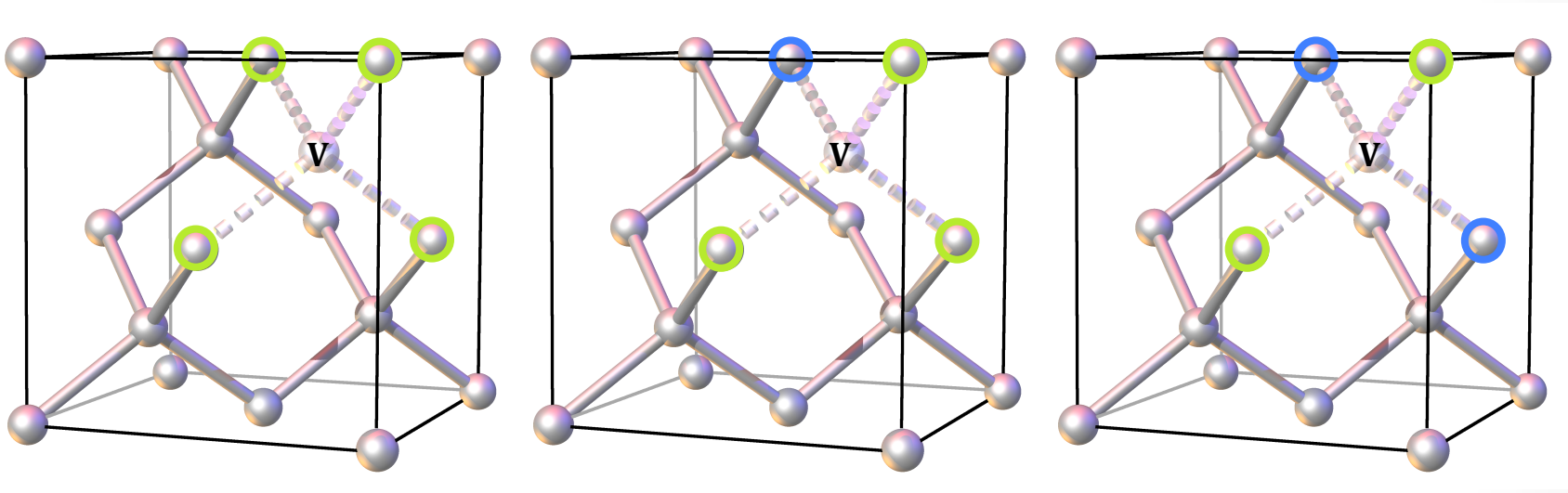

$\Psi=|\bullet\bullet\bullet\bullet>$ $\Psi=|\bullet\bullet\bullet\bullet>$ $\Psi=|\bullet\bullet\bullet\bullet>$

$S_z=2,\ T_d$ $S_z=1,\ C_{3v}$ $S_z=0,\ C_{2v}$

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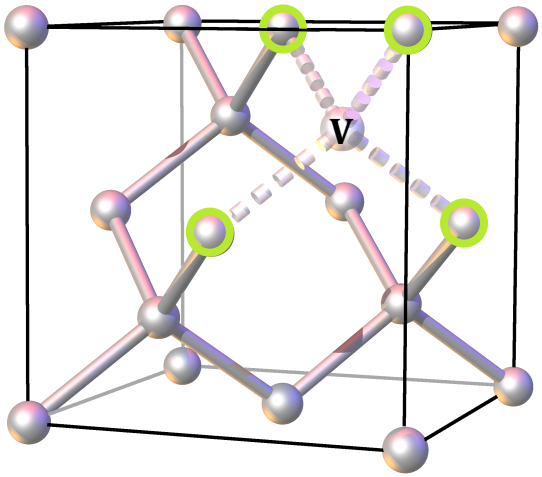

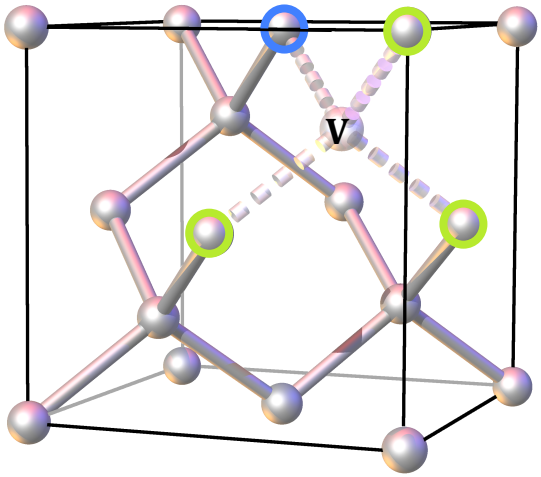

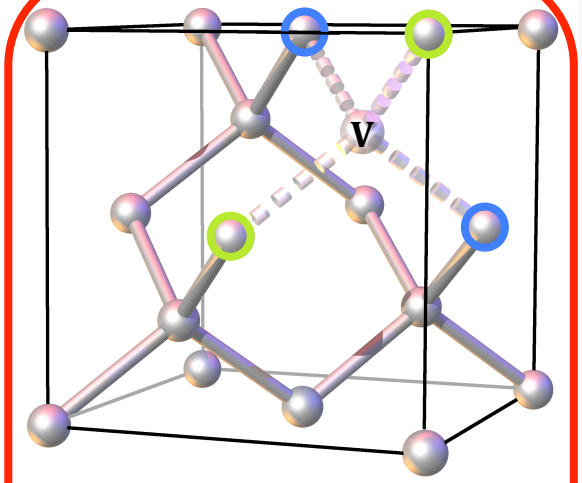

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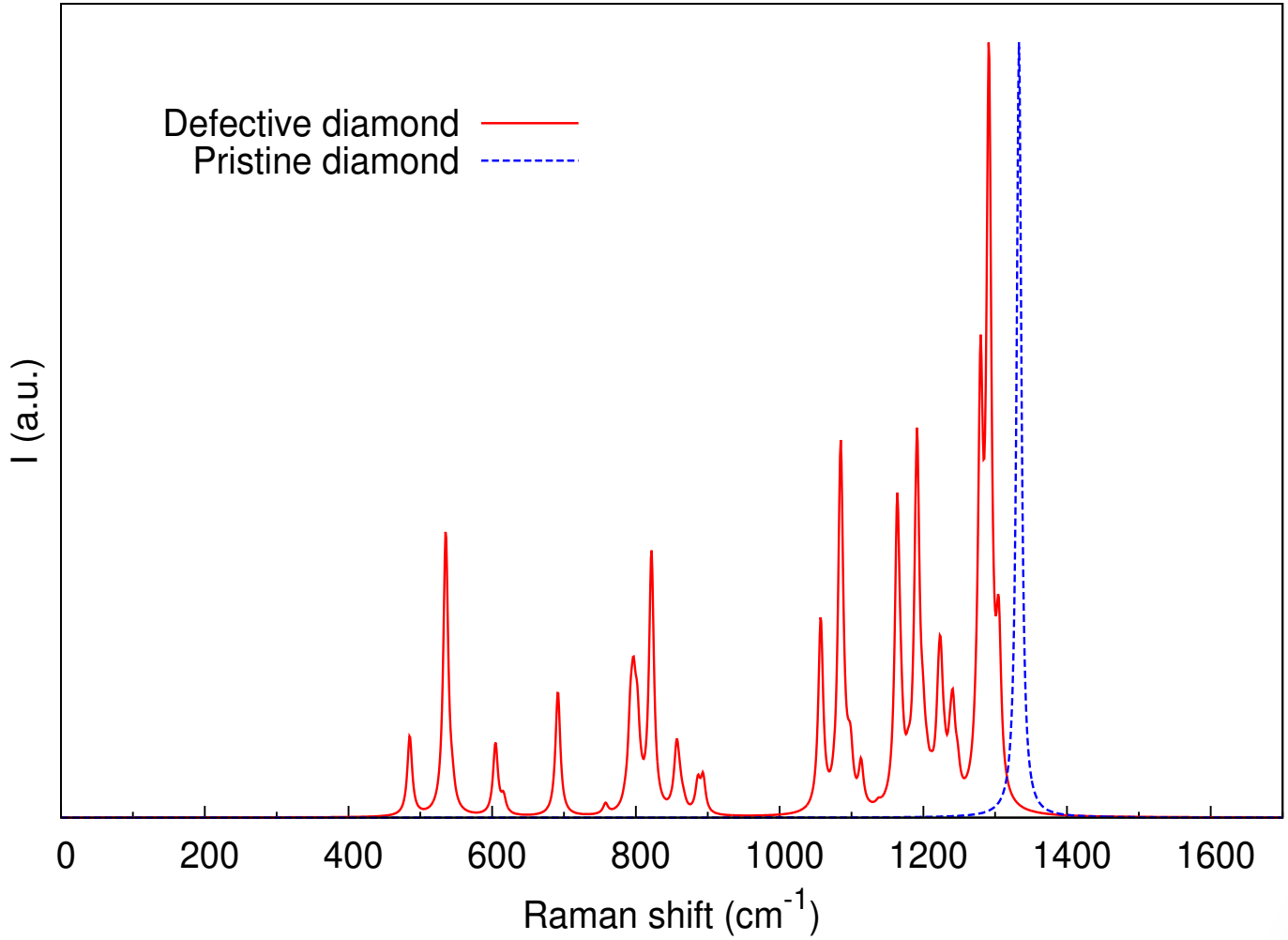
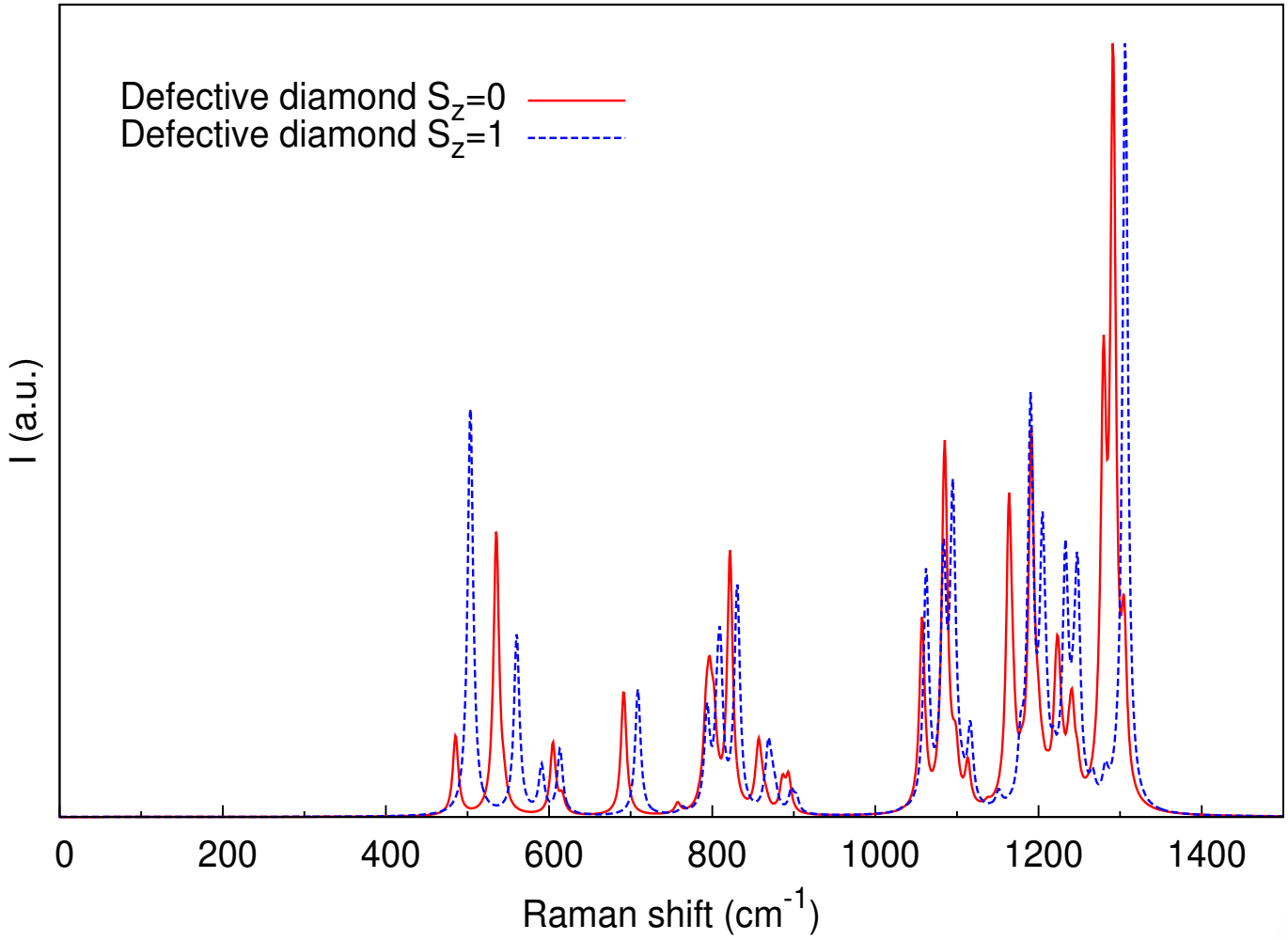
- PAULI WINS!! $E(S_z=2) > E(S_z=1) > E(S_z=0)$

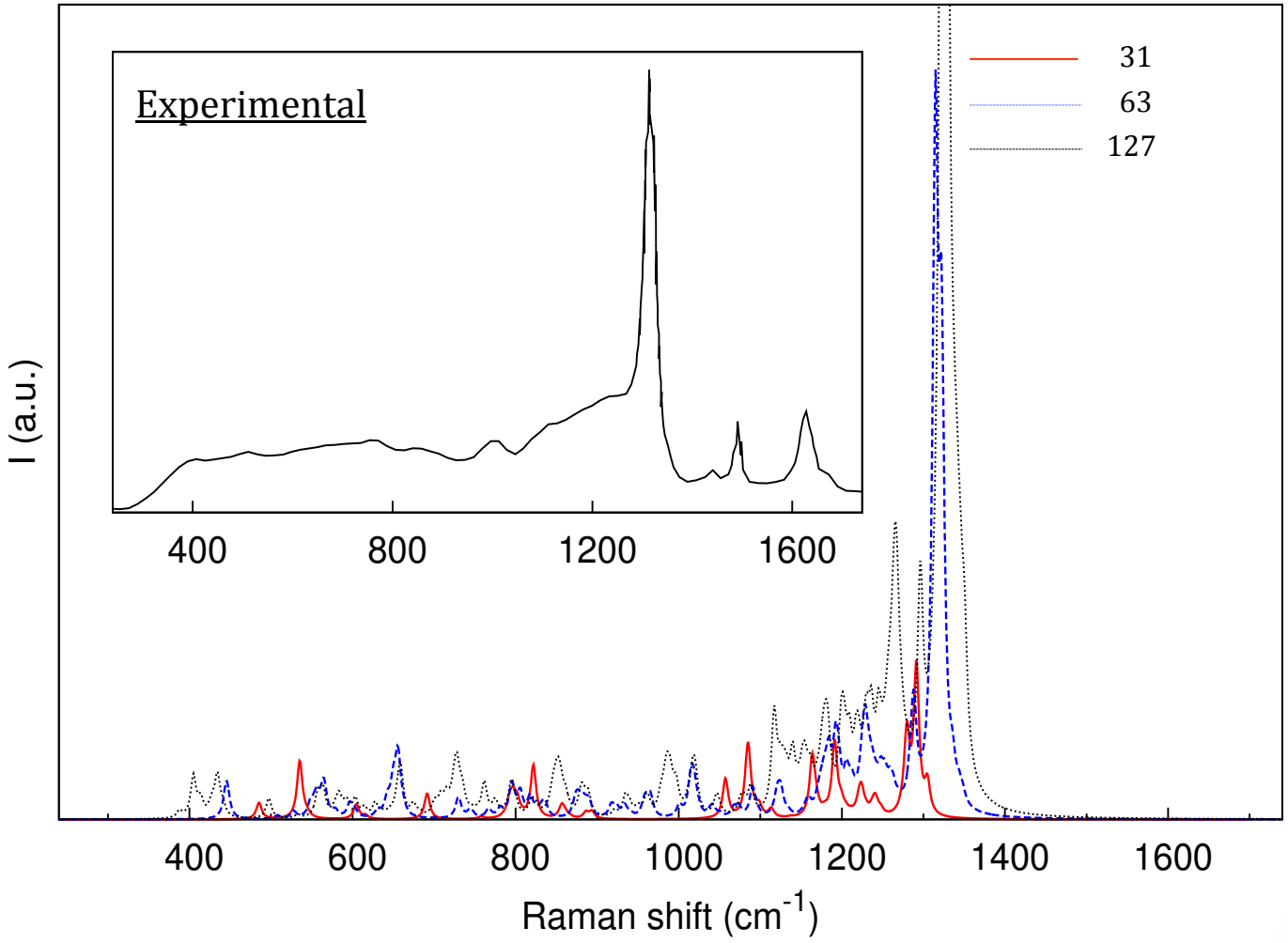
Raman Spectrum I



Raman Spectrum II



Raman Spectrum III



Papers

Zelferino, A., Salustro, S., Baima, J., Lacivita, V., Orlando, R., & Dovesi, R. (2016). Theoretical Chemistry Accounts, 135(3), 1-11.

Baima, J., Zelferino, A., Olivero, P., Erba, A., & Dovesi, R. (2016). Physical Chemistry Chemical Physics, 18(3), 1961-1968.

Thank you for your kind attention!