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SUPPORTING INFORMATION

Nitrogen Impurity States in Polycrystalline ZnO. A Combined EPR and Theoretical Study

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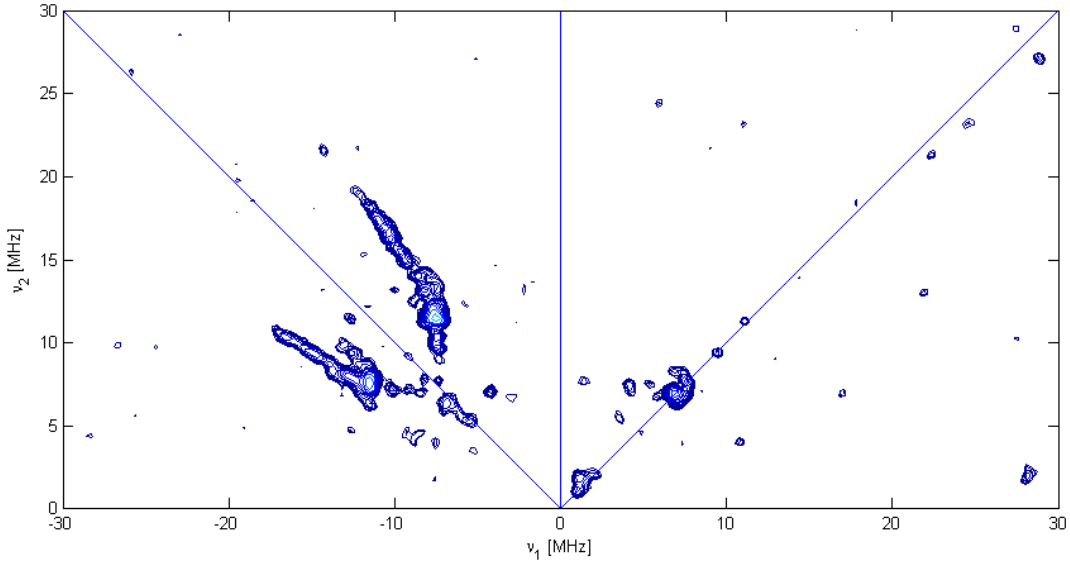

Figure S1 Normal HYSCORE spectrum recorded at B_0 = 353.2 mT
$\pi/2 - \tau - \pi/2 - t_1 - \pi - t_2 - \pi/2 - \tau$-echo with mw pulse length $t_{\pi/2}$ = 16 ns and t_π = 16 ns. The time intervals t_1 and t_2 were varied in steps of 8 ns starting from 96 ns to 3288 ns. Three different τ values (τ = 132 ns, 228 ns and 252 ns) are added together.

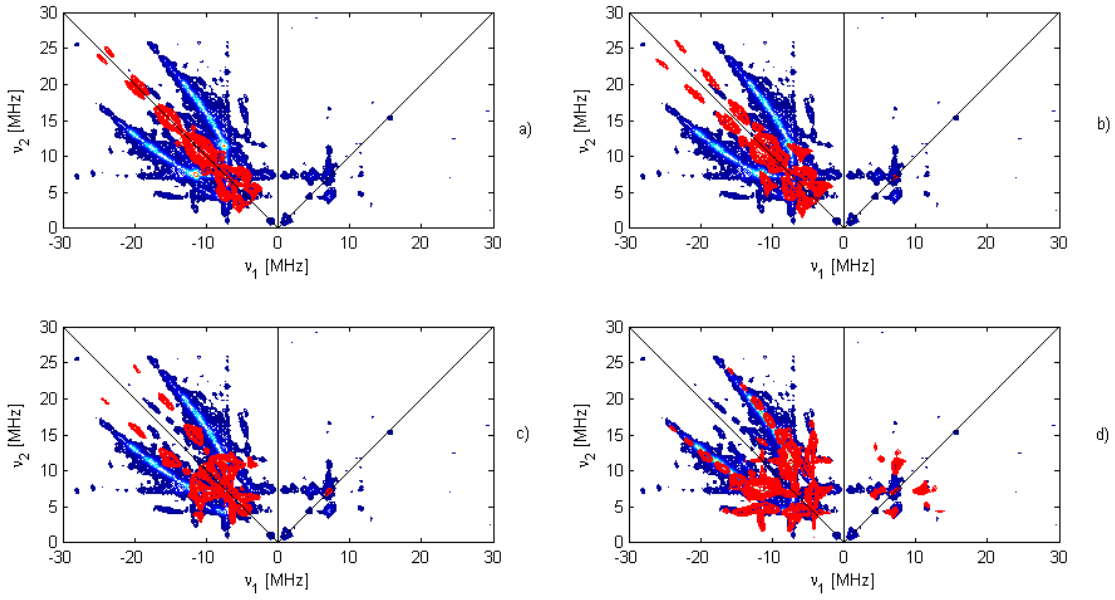

Figure S2 Simulation of the matched HYSCORE spectrum showing the effect of increasing quadrupolar interaction. a) e^2qQ/h=0, b) K=1, c) e^2qQ/h =2.5, d) e^2qQ/h =5.3 MHz. A single τ value (228 ns) was used in the simulation.

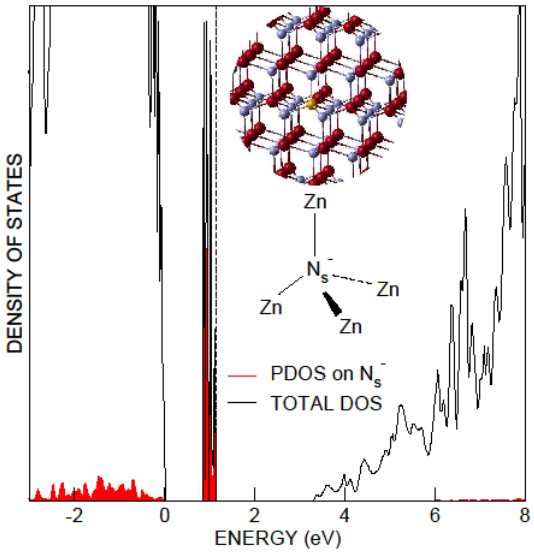

Figure S3 Total and projected (on N ion) B3LYP densities of states for the N_s^- species. The zero energy value is set at the top of the O 2p band. The dotted line indicates the Fermi energy. Insets: schematic structure of the defect centre.

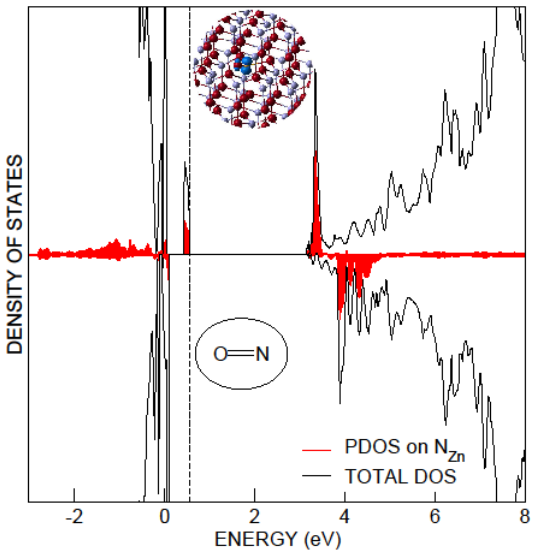

Figure S4 Total and projected (on N ion) B3LYP densities of states for the N_{Zn} species. The zero energy value is set at the top of the O 2p band. The dotted line indicates the Fermi energy. Insets: spin density plots and schematic structure of the defect centre.

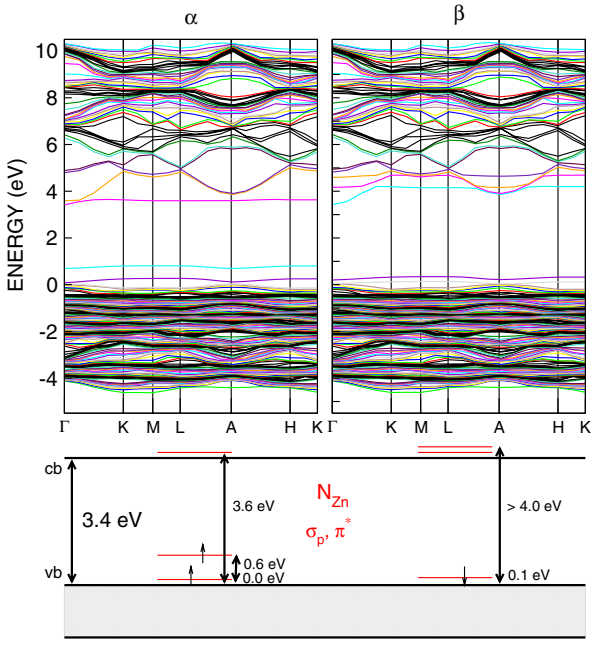

Figure S5 B3LYP electronic band structures for the N_{Zn} species.

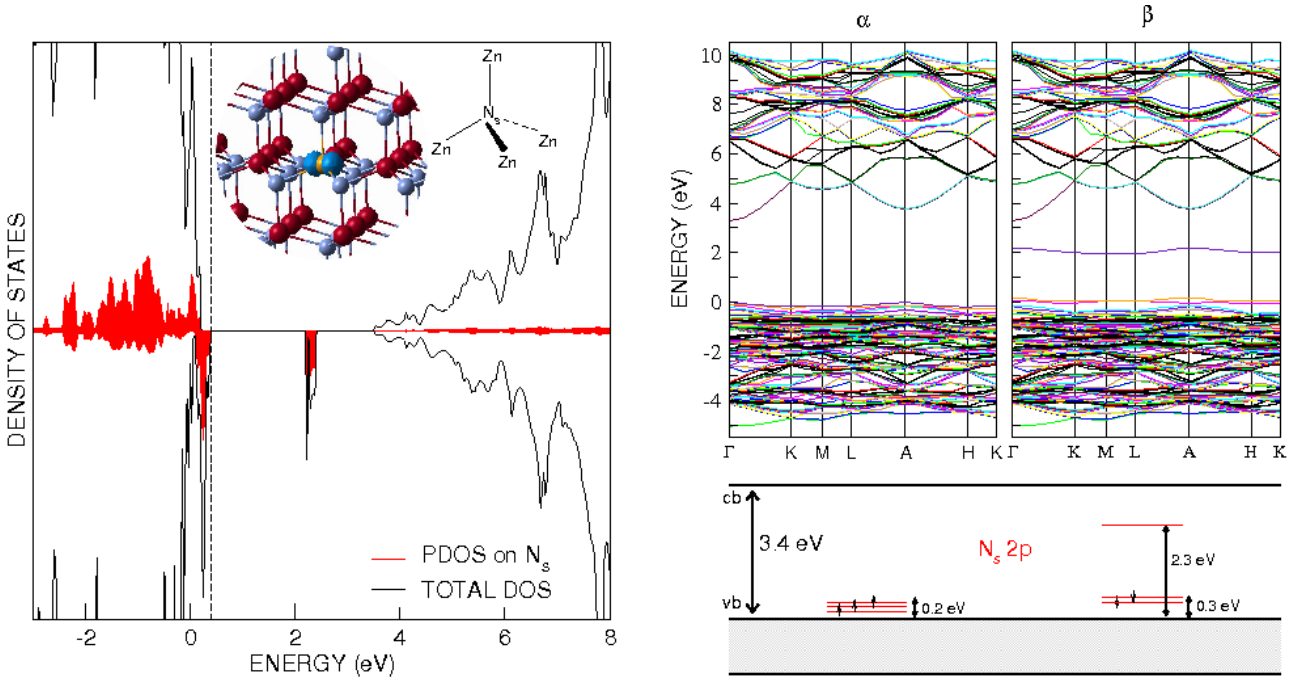

Figure S6 Total and projected (on N ion) B3LYP densities of states for the N_s isomer species with the singly occupied p-state perpendicular to the crystal c-axis. The zero energy value is set at the top of the O 2p band. The dotted line indicates the Fermi energy. Insets: spin density plots and schematic structure of the defect centre. B3LYP electronic band structures in the right panel.

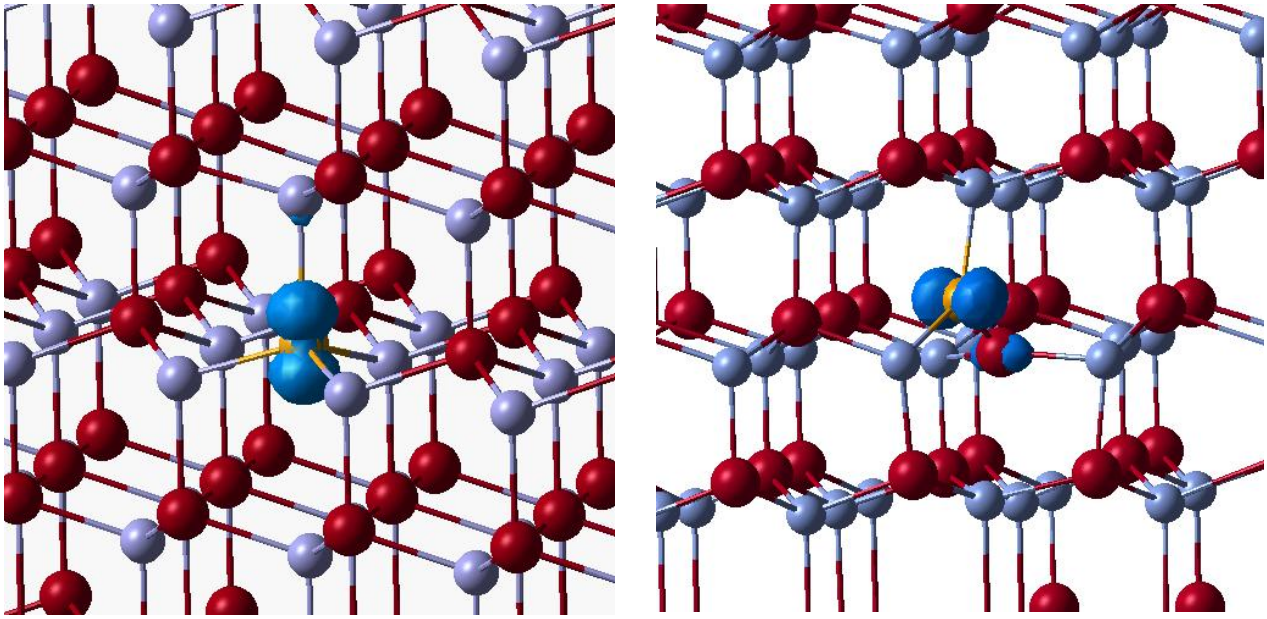

Figure S7 Spin density plots for the N_s (left) and N_{iOct} (right) species.