Electronic Supplementary Material (ESI) for Journal of Materials Chemistry
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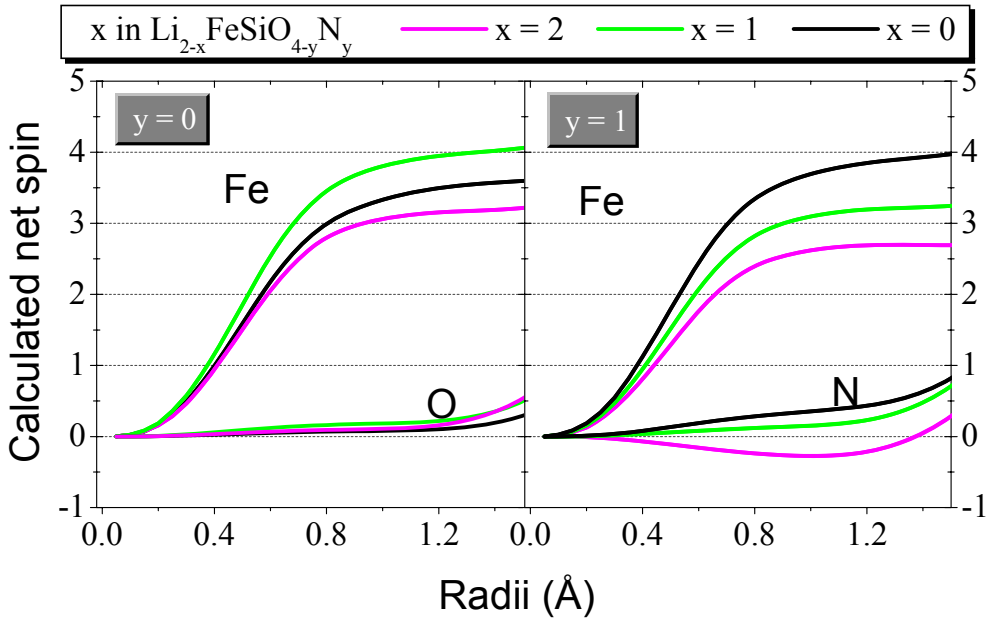
SUPPLEMENTARY INFORMATION



Conventional relaxed GGA calculations.- Integrated net spin as a function of the radius around N (O), and Fe centres in the ground states of the $Li_{2-x}FeSiO_{4-y}N_y$. Left panel Li_2FeSiO_4 (y = 0) and right panel Li_2FeSiO_3N (y =1). The lithium content (x) is represented in black (x = 0), green (x = 1) and pink (x = 2). To be compared with figure 5 in the manuscript.

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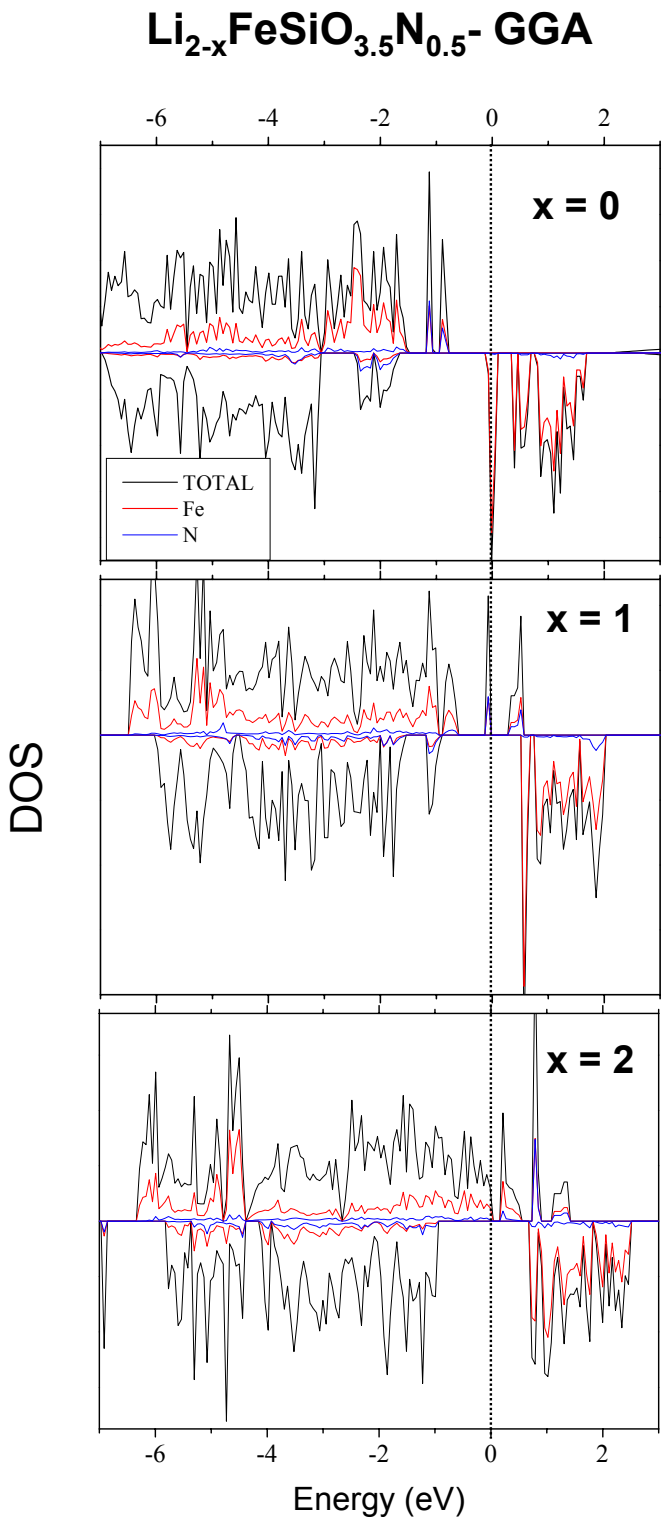

Conventional relaxed GGA calculations.- Calculated density of states (DOS) of the ground states of the $Li_{2-x}FeSiO_{3.5}N_{0.5}$ for x = 0, 1 and 2. The black lines denote the total DOS; the partial DOS of Fe and N are represented in red and blue, respectively. The zero of the energy has been set at the Fermi level. To be compared with the middle column of figure 7 in the manuscript.

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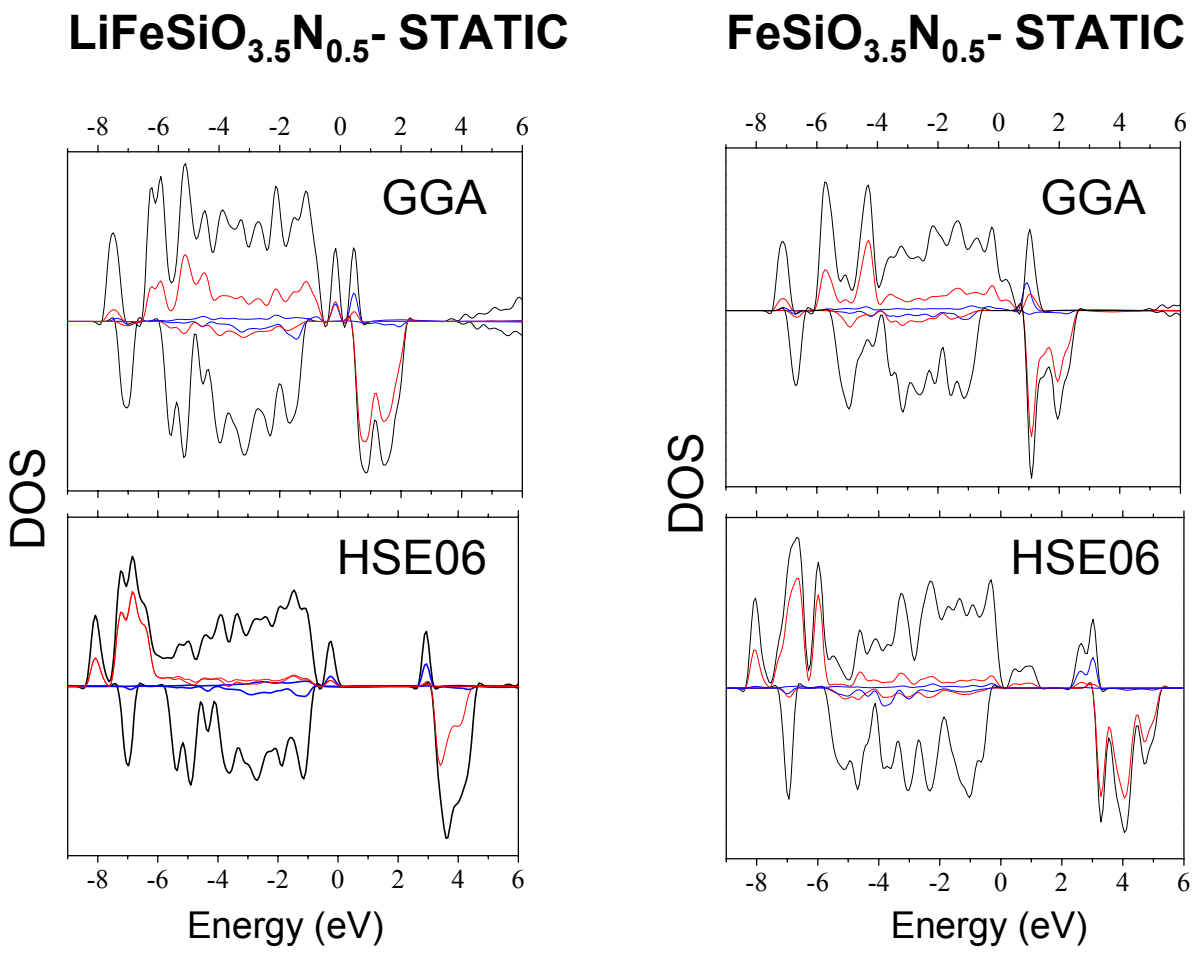

Hybrid Functional calculations.- Calculated density of states (DOS) of the ground states of $LiFeSiO_{3.5}N_{0.5}$ and $FeSiO_{3.5}N_{0.5}$ within the conventional GGA and the HSE06 hybrid functional. These static calculations were performed for the optimized structures of the relaxed-GGA+U calculations. The black lines denote the total DOS; the partial DOS of Fe and N are represented in red and blue, respectively. The zero of the energy has been set at the Fermi level.