Computer modelling of double doped $SrAl_2O_4$ for phosphor applications

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The talk will describe calculations on Sr2Al2O4, used as in phosphor applications when doped with various 2+ and 3+ cations. The calculations are used to clarify dopant sites and charge compensation mechanisms usually not mentioned in the experimental papers and will illustrate the use of potentials-based calculations in modelling point defects and dopants.

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