Title: **Cationic Diffusion in $AgBiS_2$**

Student: Ruben Marti Granero

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Supervisor: Dr. Francesc Viñes Solana
Departamento de Ciencia de Materiales y Química Física

Matildite $AgBiS_2$ has been proposed as a photoactive material for solar cells, although the disorder of the cations, Ag and Bi, is known to reduce the materials bandgap, jeopardizing its usage. The disorder mechanism is, to date, undisclosed. In the present project this is evaluated by first-principles simulations on a $AgBiS_2$ periodic bulk model, treated by Density Functional Theory (*DFT*) simulations using the Perdew-Burke-Ernzerhof (*PBE*) exchange-correlation functional. The results first show that the lineal mechanism is the first formation of Ag vacancies, which is preferred by at least 0.7 eV over the formation of either Bi or S vacancies. Once formed, the vicinal Ag atoms may diffuse to the Ag vacancies either straight or through hollow sites, with very similar energy barriers of in between 0.1-0.3 eV, while the diffusion of Bi or S is quite inhibited, which barriers of in between 1.4-2.3 eV. This correlates with an observed disordering about $\sim$ 600 K.

Keywords: Bulk, Matildite, $AgBiS_2$, Diffusion paths, Activation energies.