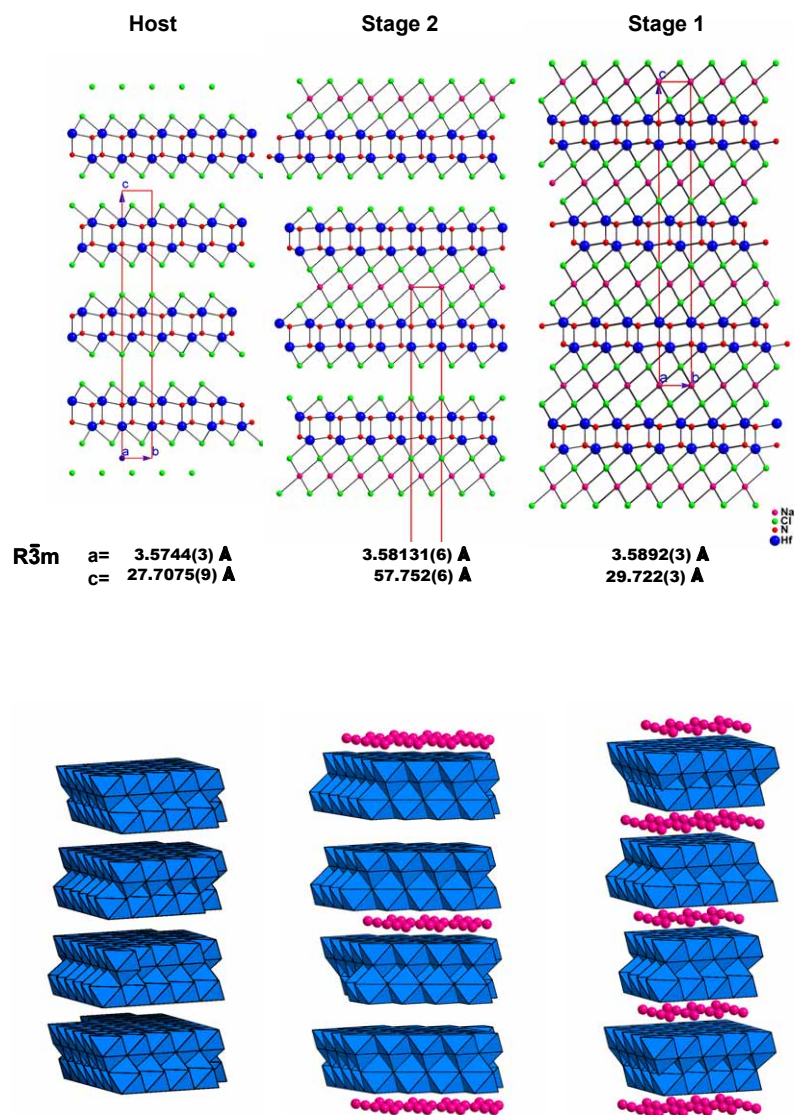


Supplementary information for the communication

*The Staging Influence on the Electronic Structure and Transport of Superconducting Sodium-doped Hafnium Nitride Chloride*

Pere Alemany, Enric Canadell and Amparo Fuyertes



Ball and stick (up) and polyhedral (bottom) representations of the crystal structures of the host and the stage 2 and stage 1 sodium intercalated phases of  $\text{HfNCl}$ ,  $\text{Na}_x\text{HfNCl}$ . Maximum occupancies of the van der Waals gaps correspond to  $x = 0.25$  for the stage 2 phase and  $x = 0.5$  for the stage 1 phase. For a stoichiometry of  $x = 0.125$  the van der Waals gaps are partly occupied in both the stage 1 and stage 2 phases.

**References:**

- (1) Fuyertes, M. Vlassov, D. Beltrán-Porter, P. Alemany, E. Canadell, N. Casañ-Pastor and M.R. Palacín, *Chem. Mater.*, 1999, 11, 203.
- (2) J. Oró-Solé, C. Frontera, B. Martínez, D. Beltrán-Porter, M. R. Palacín and A. Fuyertes, *Chem. Comm.* 2005, 3352.