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CeScSi-type intermetallics: Modulation of magnetic properties through light elements insertion and catalysis of ammonia

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The CeScSi-type structure observed for the intermetallics RETX (RE = rare-earth, T = Sc or Ti, X = Si or Ge) is an ordered variant of the La₂Sb-type that exhibits [RE₄] tetrahedral and [T₄RE₂] octahedral interstitial sites. These sites can be filled by light elements such as hydrogen, carbon or oxygen leading to modification of the physical properties.

In the first part of this presentation, we will show the effect on magnetic properties of the filling of these interstitial sites by hydrogen, carbon and oxygen. The first example concerns the insertion of C and/or H into the antiferromagnetic CeScSi parent phase [1]. The different magnetic structures were determined by neutron diffraction. Very recently, we also succeeded to insert oxygen into these intermetallic phases without decomposing them into binary or ternary oxides. The preliminary results on the structural and magnetic properties of the new phases REScSiO_x will be presented.

The second part of this communication will be devoted to the use of the CeScSi-type RETX intermetallics as Ru-supported catalysts for ammonia synthesis in the Haber-Bosch process ($N_2 + 3H_2 \rightarrow 2NH_3$). Their electride character, firstly evidenced by Hosono group in 2017 plays an important role for the dissociation of N₂ [2]. We have investigated the influence of the rare-earth (RE) element in Ru/REScSi catalysts under mild conditions (300–450 °C; 1–5 bar) [3]. Ru/CeScSi shows remarkable catalytic activity under moderate condition associated with its reversible hydrogen storage–release properties. The hydrogen desorption temperature seems to play a role as well in the catalytic activities at low temperature (300 °C). It suggests that the electride character and thus the electron donor effect can be tuned through partial hydrogenation of the REScSi materials. DFT calculations, thermodynamic and kinetic studies of hydrogen sorption are under way to answer these questions.

References

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