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THEORETICAL INSIGHT INTO METAL AND COMPLEX HYDRIDES

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Theoretical methods gain the importance as a tool for development of novel energy storage materials. The energy minimum is an objective beyond high throughput calculations, thermodynamic or structural predictions.

We summarize theoretical developments for the equilibrium surface structures of metal hydrides, like $LiNi_5$, ZrV_2 and TiFe alloys, that are crucial for their interaction with surrounding. Electrochemical and thermodynamic stability of closo and nido borates will be discussed.

References

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	Professor at Polish Academy of Sciences, former research in Denmark, Austria, Switzerland. Currently works on theoretical description of materials for energy storage and conversion, like metal oxides, metal hydrides, complex hydrides.