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Theoretical and Experimental Investigations of Binary Systems for Hydrogen Storage

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Abstract : Hydrogen is a promising energy carrier, compatible with the sustainable energy concept. In this context, solid-state hydrogen-storage is the key challenge in developing hydrogen economy. The capability of absorption of large quantities of hydrogen makes intermetallic systems of particular interest. In this study, efforts have been devoted to the theoretical investigation of binary systems with constraints consideration. On the one hand, besides considering hydrogen-storage, a reinvestigation of crystal structures of the palladium-arsenic system shows, with experimental validations, that binary systems could still currently present new or unknown relevant structures. On the other hand, various binary Mg-based systems were theoretically scrutinized in order to find new interesting alloys for hydrogen storage. Taking the effect of pressure into account reveals a wide range of alternative structures, changing radically the stable compounds of studied binary systems. Similar constraints, induced by Pulsed Laser Deposition, have been applied to binary systems, and results are presented.

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