National Institute of Technology Rourkela

Departmental Seminar

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| Seminar Title | : Prediction of Hydrogen Storage in Metal and Complex Hydrides: A Supervised Machine Learning Approach |
| Speaker | : Rama Chandra Muduli |
| Supervisor | : Prof. Paresh Kale (2447) |
| Venue | : UG Seminar Room |
| Date and Time | : 20 Feb 2025 (10:30) |
| Abstract | : Hydrogen storage technology is crucial for the rapidly expanding hydrogen-based energy infrastructure, production, and delivery. Among the numerous efforts to develop safe hydrogen storage solutions, solid-state hydrogen storage using metal hydrides is widely favored due to its high hydrogen storage capacity (e.g., MgH~7 wt.% and LiH~12.6 wt.%) and significant reaction kinetics. However, developing a solid-state storage system is challenging due to the effect of numerous parameters. The metal hydrides examined for hydrogen storage exhibit varying storage capacities and hydrogen absorption and desorption kinetics, depending on the operating temperature and pressure. In this study, various machine learning (ML) models were developed based on the most sensitive parameters for determining hydrogen storage capacity: charging pressure and temperature. The work reports the prediction of hydrogen storage in IMCs (AB, A2B, AB2, and AB5), Mg, MIC (miscellaneous intermetallic compounds), SS (solid solutions), and complex compounds using supervised machine learning. The publicly available hydride database for hydrogen storage by the US Department of Energy was analyzed. Regression methods such as linear regression, polynomial regression, decision tree regression, and random forest regression were employed to compare the accuracy of hydrogen storage predictions. The performance of the ML models was compared to previously reported studies, with the decision tree regression model showing superior results, achieving a coefficient of determination of 0.93 and a mean square error of 0.19. The decision tree regression offers improved $R^2$ and additional advantages, such as simplicity, ease of interpretation, no requirement for feature scaling, and the capability to capture non-linear relationships. |