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AI predicts the precursor materials needed for material synthesis

Researchers in Korea have developed a technology that automatically identifies the necessary precursor materials to synthesize specific target materials. A joint research team led by Senior Researcher Gyoung S. Na from the Korea Research Institute of Chemical Technology (KRICT) and Professor Chanyoung Park from the Korea Advanced Institute of Science and Technology (KAIST) has developed an AI-based retrosynthesis methodology that predicts the required precursor materials solely based on the chemical formula of the target material without expensive material descriptors and chemical analysis.

Precursor materials refer to all essential materials required in the synthesis process of the desired target material. In recent years, materials discovery has become a crucial task across various industries, including batteries and semiconductors. Traditionally, finding the right intermediate materials for synthesis has required costly and repetitive experiments. However, there is a growing demand for utilizing AI to identify these materials efficiently.

The research team developed an innovative AI technology that can learn the inverse process of predicting the necessary precursor materials of the target material using only its chemical formula. This newly developed technology overcomes the challenges posed by the complex 3D structures of inorganic materials, such as atomic arrangements and bonding information. Instead, the AI analyses the types and ratios of elements present in the target material and calculates the thermodynamic formation energy differences to identify precursors that facilitate easier synthesis reactions.

To improve the accuracy of precursor material predictions, the team employed a deep neural network specialized in chemical data. The AI model was trained on approximately 20,000 published research papers detailing material synthesis processes and precursor materials. The AI model was tested on around 2,800 synthesis experiments that were not provided in the training dataset. The evaluation results showed that it successfully predicted the necessary precursor materials in over 80% of cases within just 0.01 seconds by utilizing GPU acceleration. (Source: Heewoong Noh et al, *arXiv* (2024).