Marking Criteria: Energy Modeling and Structural Analysis of Gold Clusters

The competition will be evaluated based on the following detailed scoring criteria. Each team must submit a 20-page limit report summarizing their model and methodology, explaining the application scenarios and potential impact of the prediction results. All aspects of submission count toward the 20-page limit (Summary Sheet, Table of Contents, Reference List, and any Appendices）

Task 1 — Predicting Energies of Au_{20} Clusters	**Data Understanding and Preprocessing (8%)** • Correct parsing of .xyz files • Detection and handling of data issues • Brief statistical summary of the dataset • Visualization of example structures using molecular viewers such as VMD **Feature Extraction and Representation (12%)** • Design of meaningful structural descriptors • Application of dimensionality reduction or feature selection where relevant • Explanation of physical relevance between selected features and energy prediction **Model Construction and Evaluation (10%)** • Selection of suitable modeling approach with clear justification • Reporting of performance metrics: MAE, RMSE, R^2 • Discussion of model strengths and limitations	30%
Task 2 — Finding and Describing the Most Stable Shapes	• Statistical analysis of energy distribution (mean, variance, skewness) • Correct identification of the lowest-energy structure • Visualization of the identified structure with clear labeling • Scientific description of structural features (e.g., symmetry, bond lengths, geometry)	20%
Task 3 — Sensitivity Analysis via Local Structural Perturbation	• Creation of perturbed structures from the lowest-energy reference found in Problem 2 • Energy predictions for perturbed structures using the model from Problem 1 • Calculation of energy differences compared to the original structure (MAE, RMSE) • Discussion of model sensitivity and stability with respect to local changes	20%
Innovation and Creativity	• Novel feature engineering or modeling approaches • Unique visualization or analysis methods • Original insights into energy–structure relationships or model behavior	20%

Report Quality	• Clarity and comprehensiveness of the one-page report summarizing the model • Logical structure, clear writing, and accurate terminology • Proper integration of figures, tables, and explanations • Explicit statements of methods, assumptions, and results • Correct citations and acknowledgments	10%