Section	Criteria	Points
1. Implementation (60 Points)		
	A. Grand Canonical Monte Carlo Simulation (40 Points)	
	Correct Initialization of the 2D Lattice – Properly sets up a 2D square lattice – Initializes lattice sites (*e.g.*, as empty or occupied)	10
	Implementation of Adsorption and Desorption Moves – Correctly codes the adsorption of nitrogen and hydrogen – Implements desorption moves	10
	Acceptance Criteria Using the Metropolis Algorithm – Accurately calculates the change in grand potential for moves – Applies the Metropolis criterion for move acceptance	10
	Handling of Interaction Energies Between Species – Incorporates interaction energies (ϵ_{NN}, ϵ_{HH}, ϵ_{NH}) – Ensures interactions affect the adsorption/desorption processes correctly	10
	B. Use of Provided Pseudocode and Code Snippet (10 Points)	
	Adherence to Pseudocode Structure – Follows the logical flow outlined in the pseudocode – Adapts the pseudocode appropriately to the problem specifics	6
	Effective Use of Code Snippet for Testing – Utilizes the snippet to verify implementation correctness – Demonstrates understanding by modifying and expanding the snippet as needed	4
	C. Simulation of Parameter Sets (10 Points)	
	Correctly Simulates Each Parameter Set (2 Points Each) – Ideal Mixture of Nitrogen and Hydrogen – Repulsive Interactions between Nitrogen and Hydrogen – Attractive Interactions between Nitrogen and Hydrogen – Immiscible Nitrogen and Hydrogen – "Like Dissolves Unlike" Scenario	10
2. Phase Diagrams (50 Points)		
	A. Exploration of Parameter Space (10 Points)	
	Use of Provided `mus_A` and `Ts` Arrays – Correctly implements the arrays to vary μ_{H} and T – Explores a sufficient range to capture different phases	6

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Section	Criteria	Points
	Efficient Parameter Space Exploration – Ensures simulations run efficiently without unnecessary computations – Uses appropriate step sizes in the arrays	4
	B. Generation of Phase Diagrams (30 Points)	
	Plotting Mean Coverage vs. μ_{H} and T – Accurate plots for nitrogen coverage (4 Points) – Accurate plots for hydrogen coverage (4 Points) – Accurate plots for total coverage (4 Points)	12
	Inclusion of Color Bars Indicating Coverage Values – Color bars included in all phase diagrams (4 Points) – Proper labeling and scaling of color bars (4 Points)	8
	Clarity and Presentation of Phase Diagrams – Axes labeled with correct units and variables (4 Points) – Legible legends and titles for all plots (4 Points) – Consistent formatting across all diagrams (2 Points)	10
	C. Lattice Configurations Visualization (10 Points)	
	Visual Representation for Each Parameter Set – Clear images showing lattice states (4 Points) – Visualization highlights differences between parameter sets (6 Points)	10
3. Analysis. (50 Points)		
	A. Adsorption Behavior Analysis (20 Points)	
	Discussion of Nitrogen and Hydrogen Adsorption – Insightful interpretation of nitrogen adsorption trends (6 Points) – Insightful interpretation of hydrogen adsorption trends (6 Points)	12
	Adsorption Under Different Conditions – Analyzes how temperature and chemical potential affect adsorption – Explains observed phenomena using thermodynamic principles	8
	B. Comparison Between Parameter Sets (20 Points)	
	Identification of Key Differences – Highlights how interaction energies influence adsorption – Compares coverage levels across different scenarios	12
	Explanation of Observed Differences – Provides theoretical justification for differences	8

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Section	Criteria	Points
	– References specific data from simulations	
	C. Implications for Ammonia Synthesis (10 Points)	
	Connection to Industrial Process – Explains how adsorption behavior impacts ammonia production – Relates findings to catalyst efficiency and reaction rates	6
	Optimization Strategies – Suggests methods to enhance ammonia synthesis based on results – Considers practical implementation in industrial settings	4
4. Report (30 Points)		
	A. Quality of Writing (10 Points)	
	Clarity and Conciseness – Presents information logically and coherently – Avoids unnecessary jargon and explains technical terms	4
	Grammar and Spelling – Minimal grammatical errors – Proper punctuation and spelling throughout	2
	Structure and Organization – Includes introduction, methodology, results, discussion, conclusion – Uses headings and subheadings effectively	4
	B. Inclusion of Figures and Lattice Configurations (10 Points)	
	All Required Figures Included – Phase diagrams for each parameter set – Lattice configuration images where appropriate	6
	Figure Quality and Formatting – High-resolution images – Figures are properly labeled and referenced in the text	4
	C. Physical Interpretation and Implications (10 Points)	
	Explanation of Results – Interprets simulation data in the context of physical chemistry – Discusses the significance of adsorption patterns	6
	Implications for Ammonia Synthesis Process – Links simulation outcomes to real-world applications	4

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Section	Criteria	Points
	– Provides thoughtful insights into industrial relevance	
5. Submission (10 Points)		
	A. GitHub Repository (6 Points)	
	Code Organization and Documentation – Code is well-organized into directories/files – Includes comments and documentation for understanding	4
	Report Inclusion – Report is included in the repository as a PDF	2
	B. Submission of Repository Link (4 Points)	
	Timely Submission – Repository link submitted before the deadline	2
	Accessibility – Repository is public – Link directs to the correct repository	2