SNS COLLEGE OF PHARMACY AND HEALTH SCIENCES

Affiliated To The Tamil Nadu Dr. MGR Medical University, Chennai Approved by Pharmacy Council of India, New Delhi.

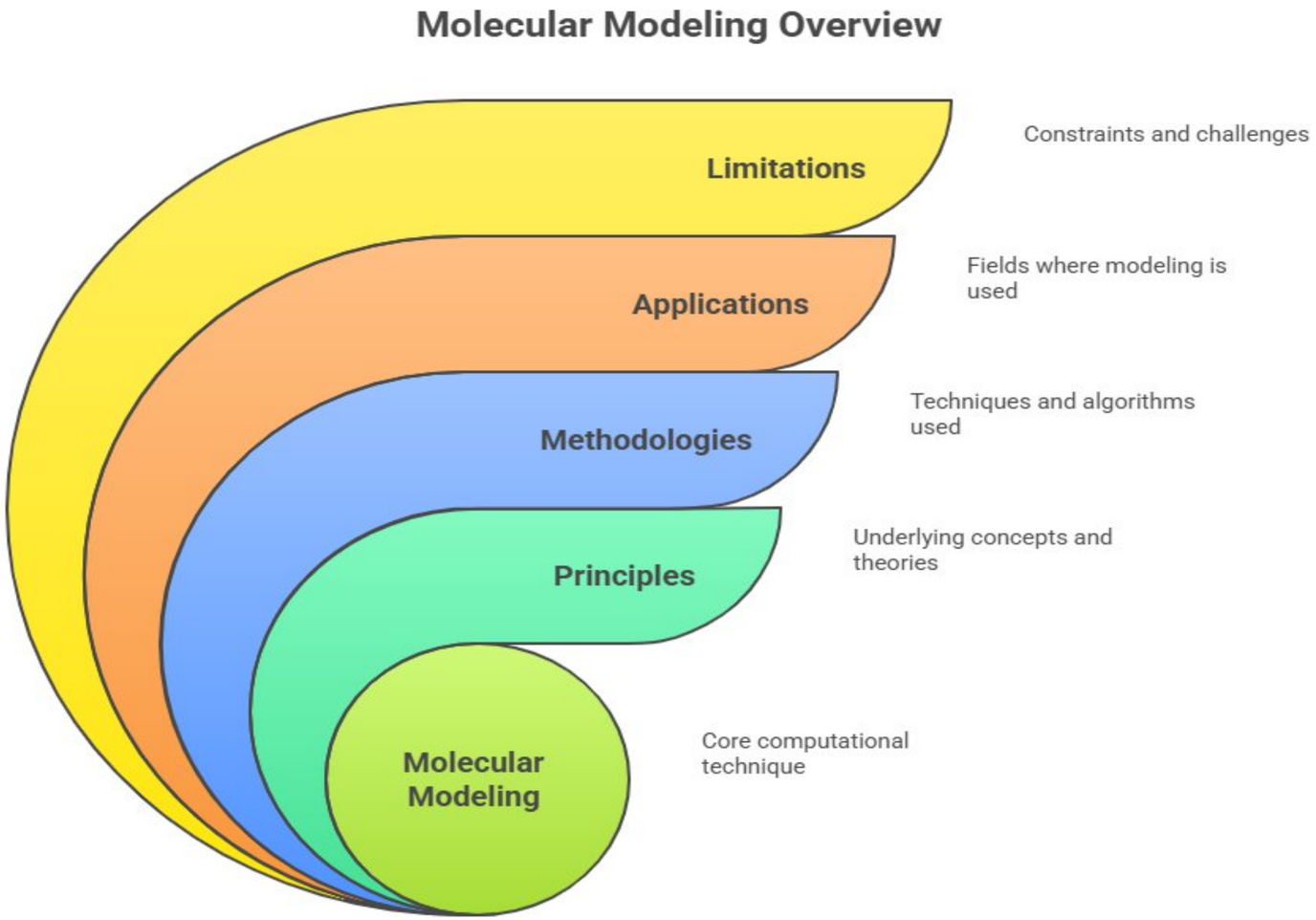
Coimbatore -641035

COURSE NAME : COMPUTER AIDED DRUG DESIGN(BP 807 ET)

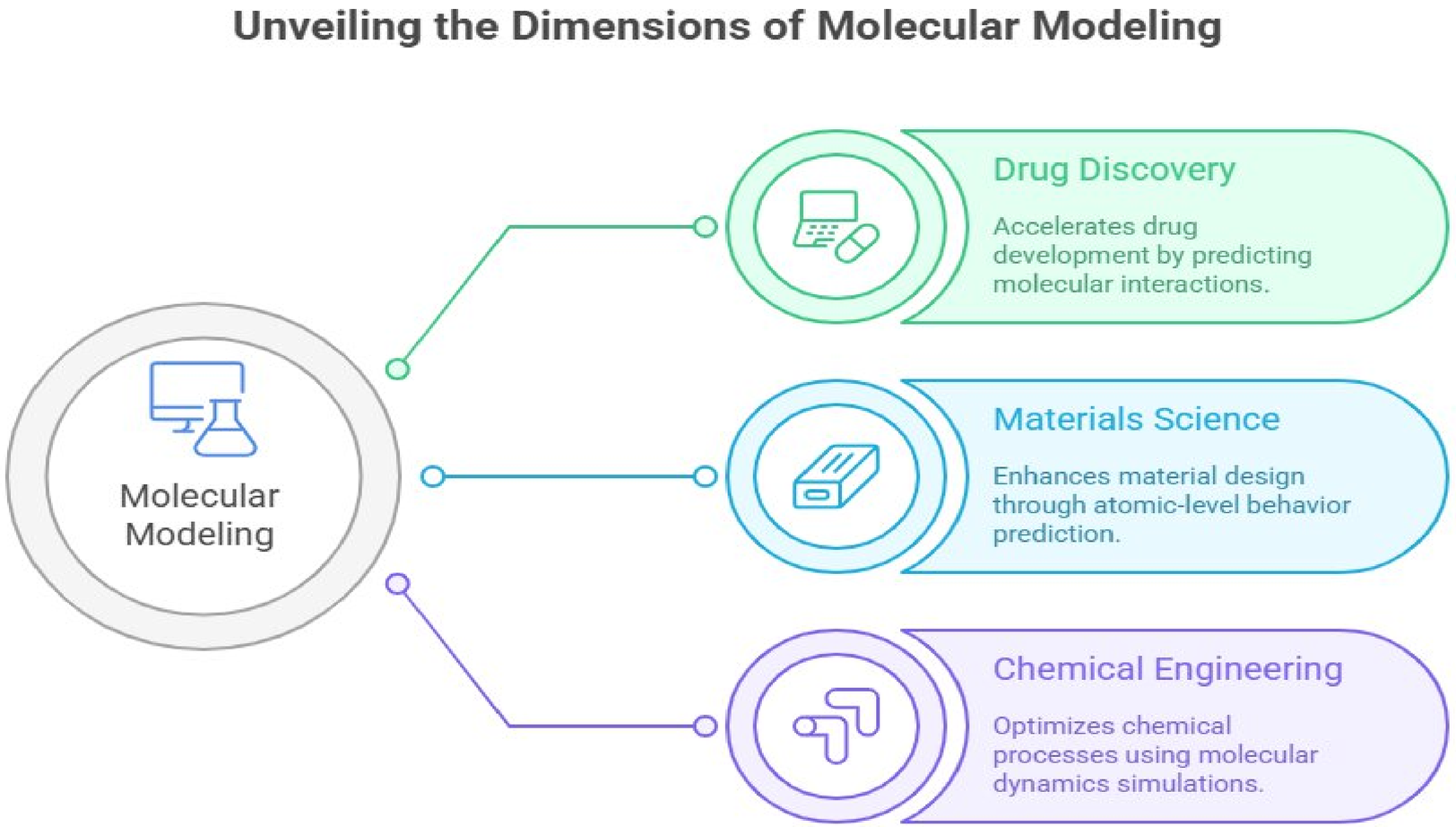
VIIISEM / IV YEAR

TOPIC: MOLECULAR MODELING

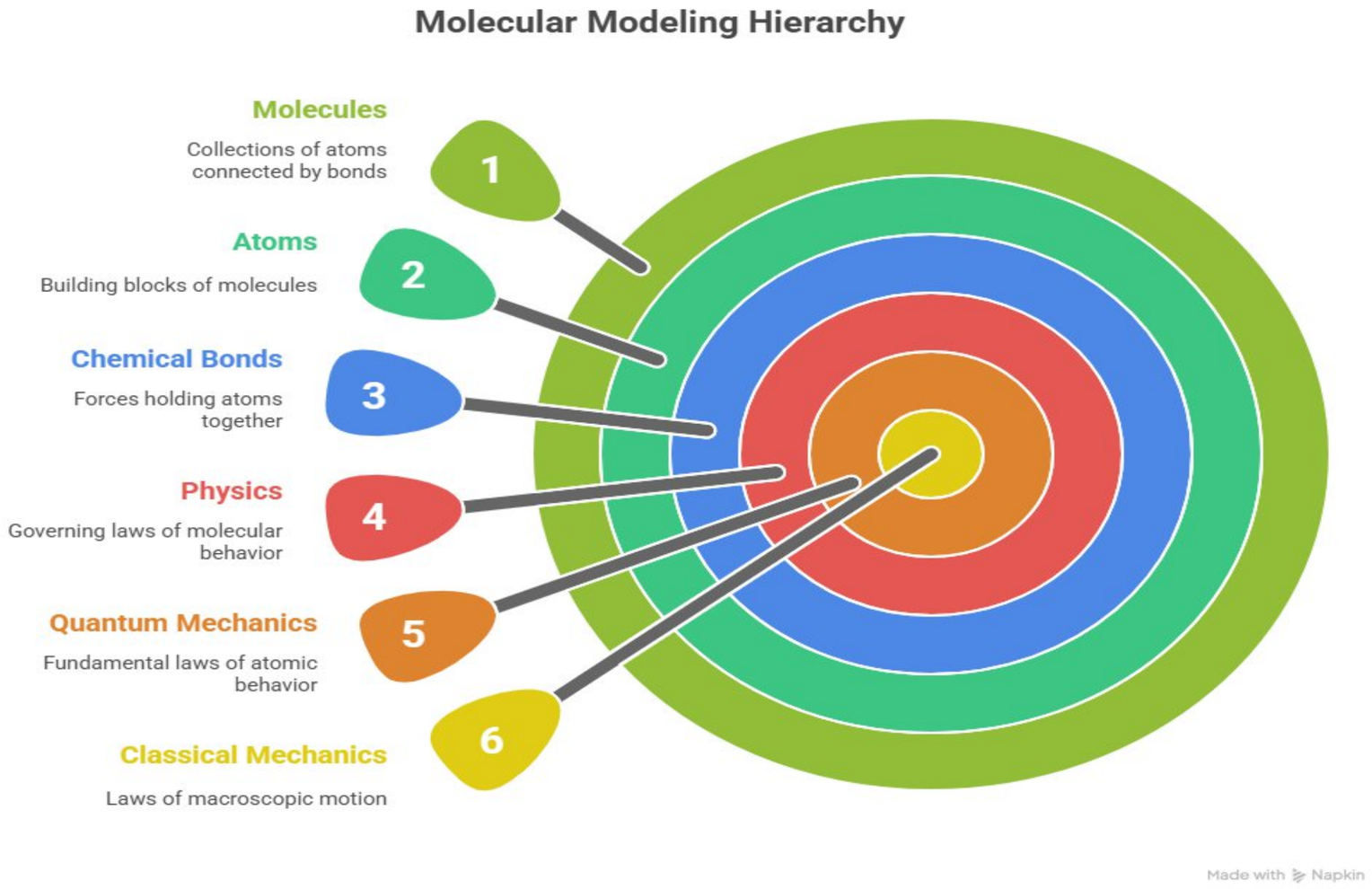
MOLECULAR MODELING OVERVIEW



INTRODUCTION



PRINCIPLES


Molecular Modeling Hierarchy
Molecules
Collections of atoms connected by bonds
1
Atoms
Building blocks of molecules
2
Chemical Bonds
Forces holding atoms together
3
Physics
Governing laws of molecular behavior
4
Quantum Mechanics
Fundamental laws of atomic behavior
5
Classical Mechanics
Laws of macroscopic motion
6
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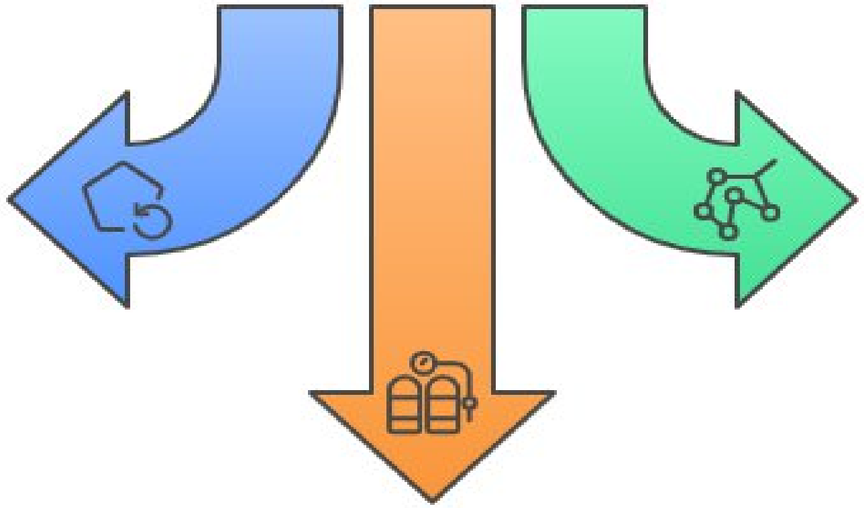
METHODOLOGY

Which molecular modeling methodology should be used?



Molecular Dynamics

Explores time-dependent behavior of molecular systems.

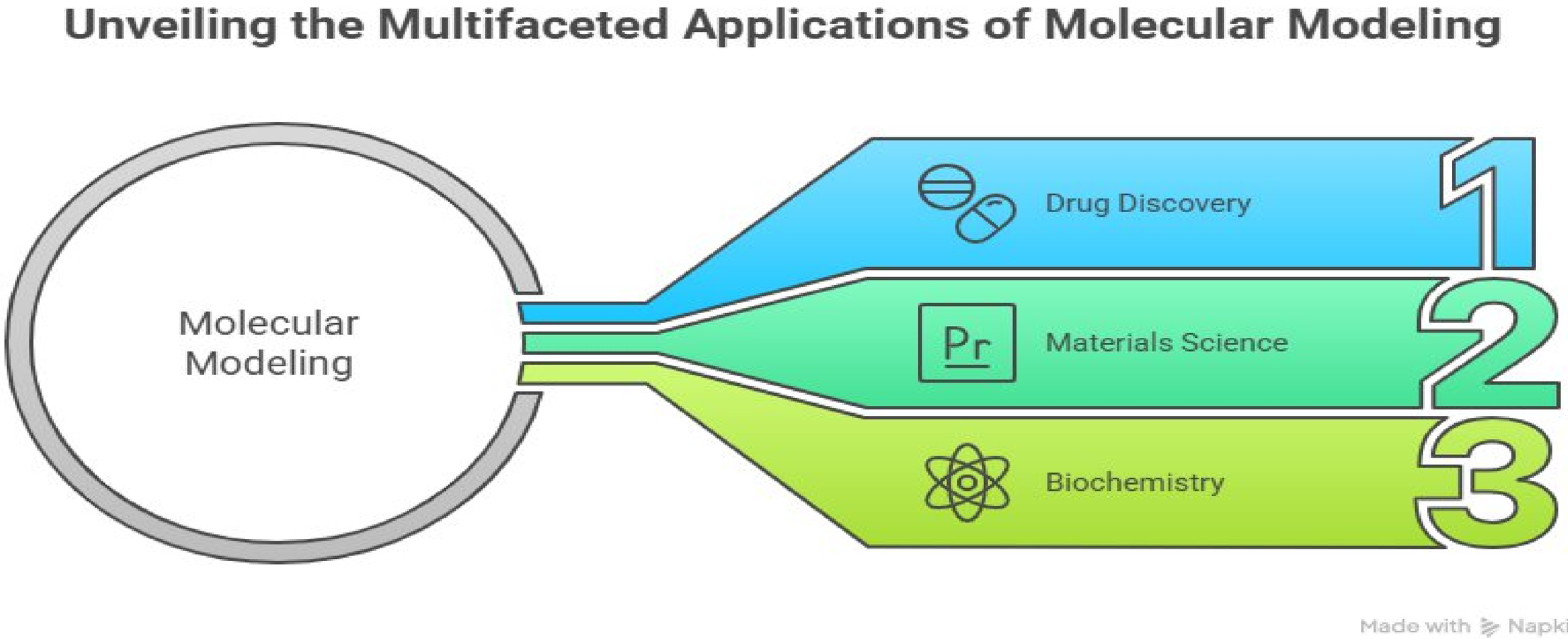
Quantum Mechanics

Provides insights into electronic structures and properties.

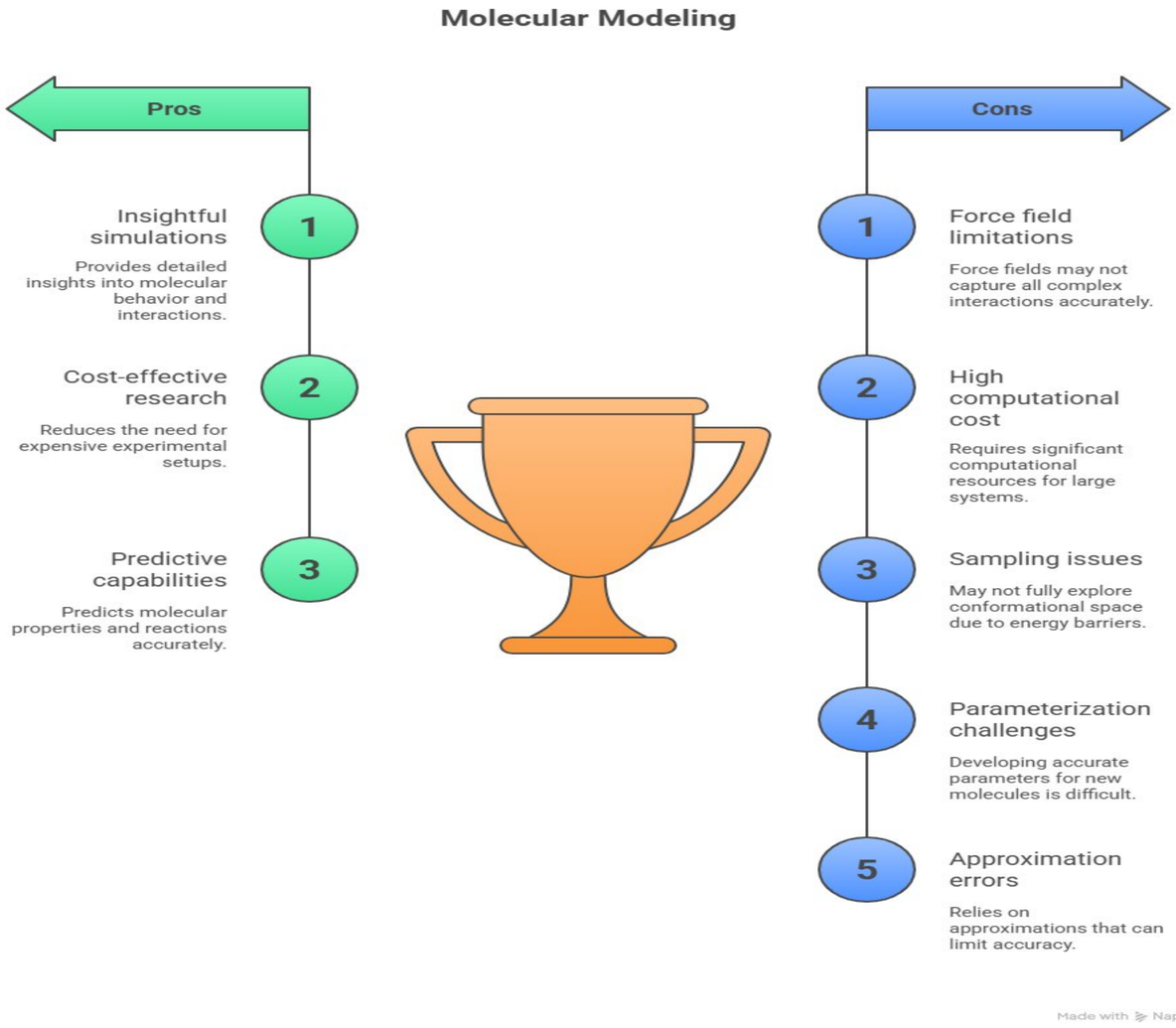
Docking Studies

Predicts molecular interactions.

APPLICATIONS



LIMITATIONS



FUTURE DIRECTIONS

Molecular Modeling Advancements

Experimental Data Integration

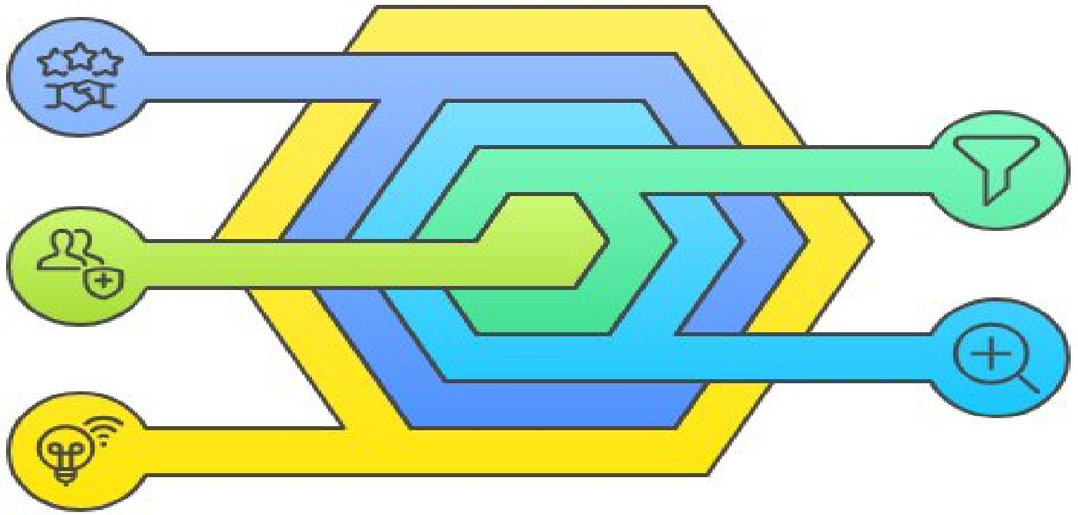
Combining simulation and reality

Accurate Force Fields

Core of molecular simulations

New Application Areas

Expanding molecular modeling's reach



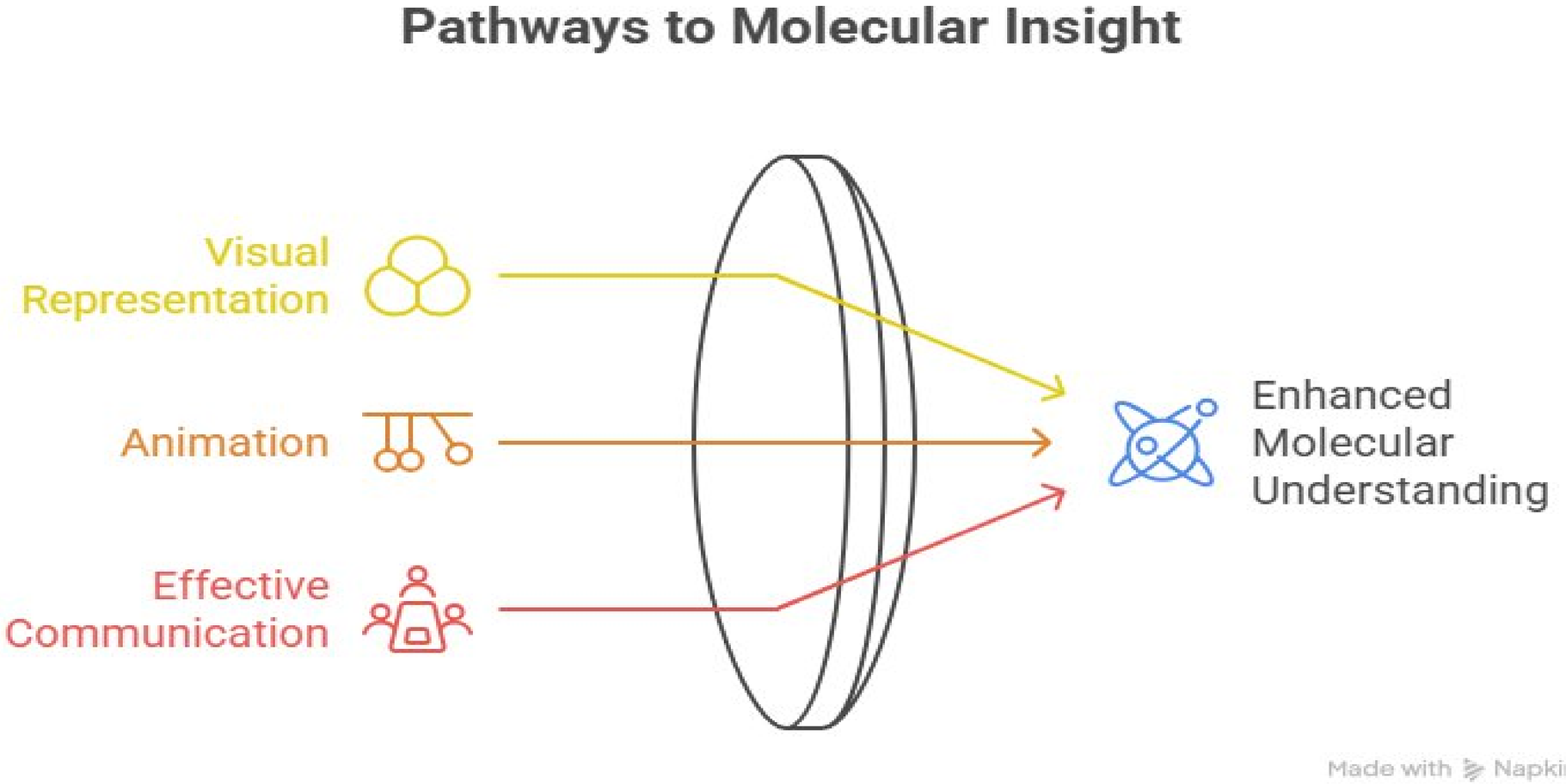
Efficient Sampling Methods

Overcoming energy barriers

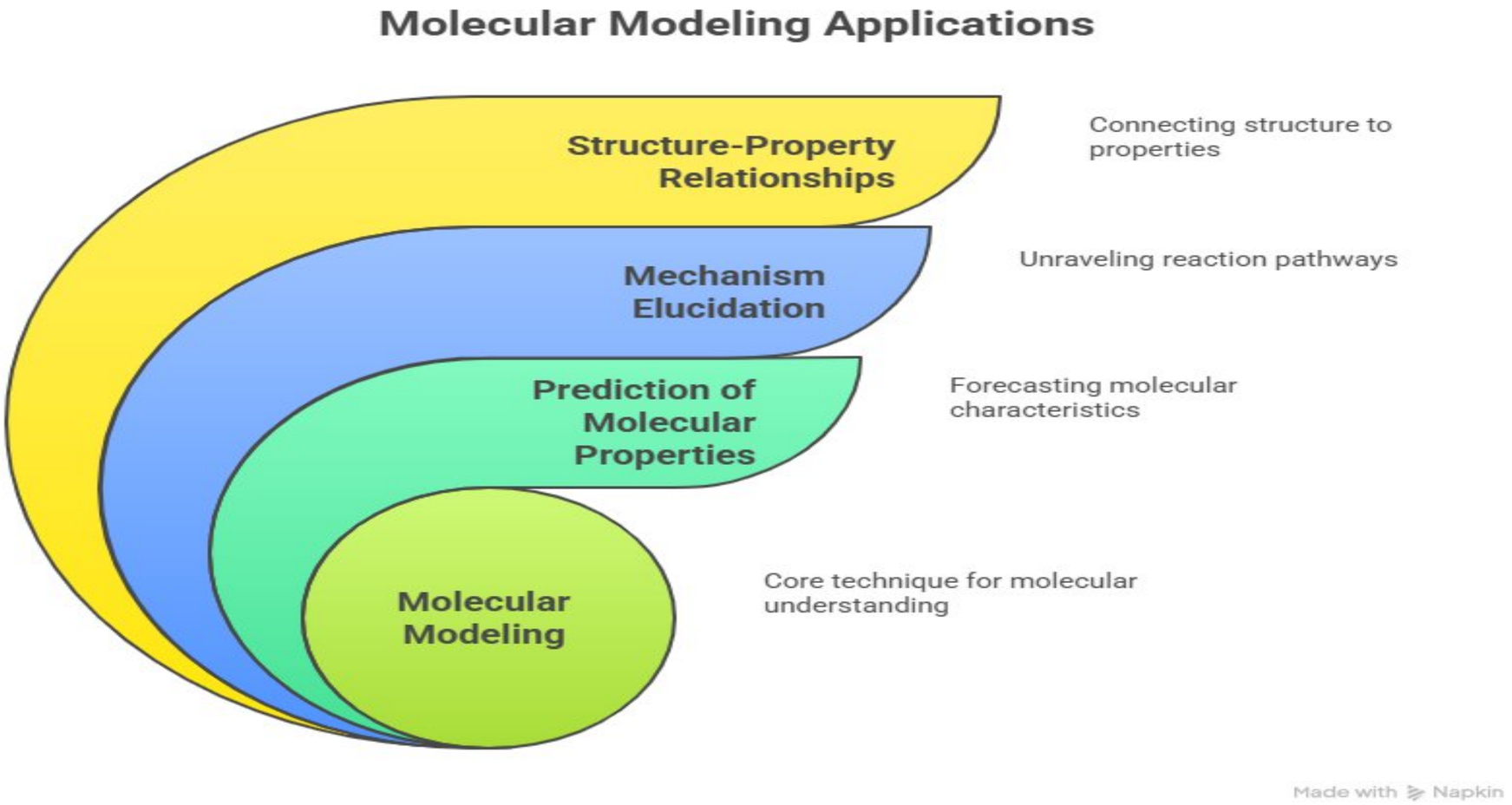
Scalable Algorithms

Simulating large systems

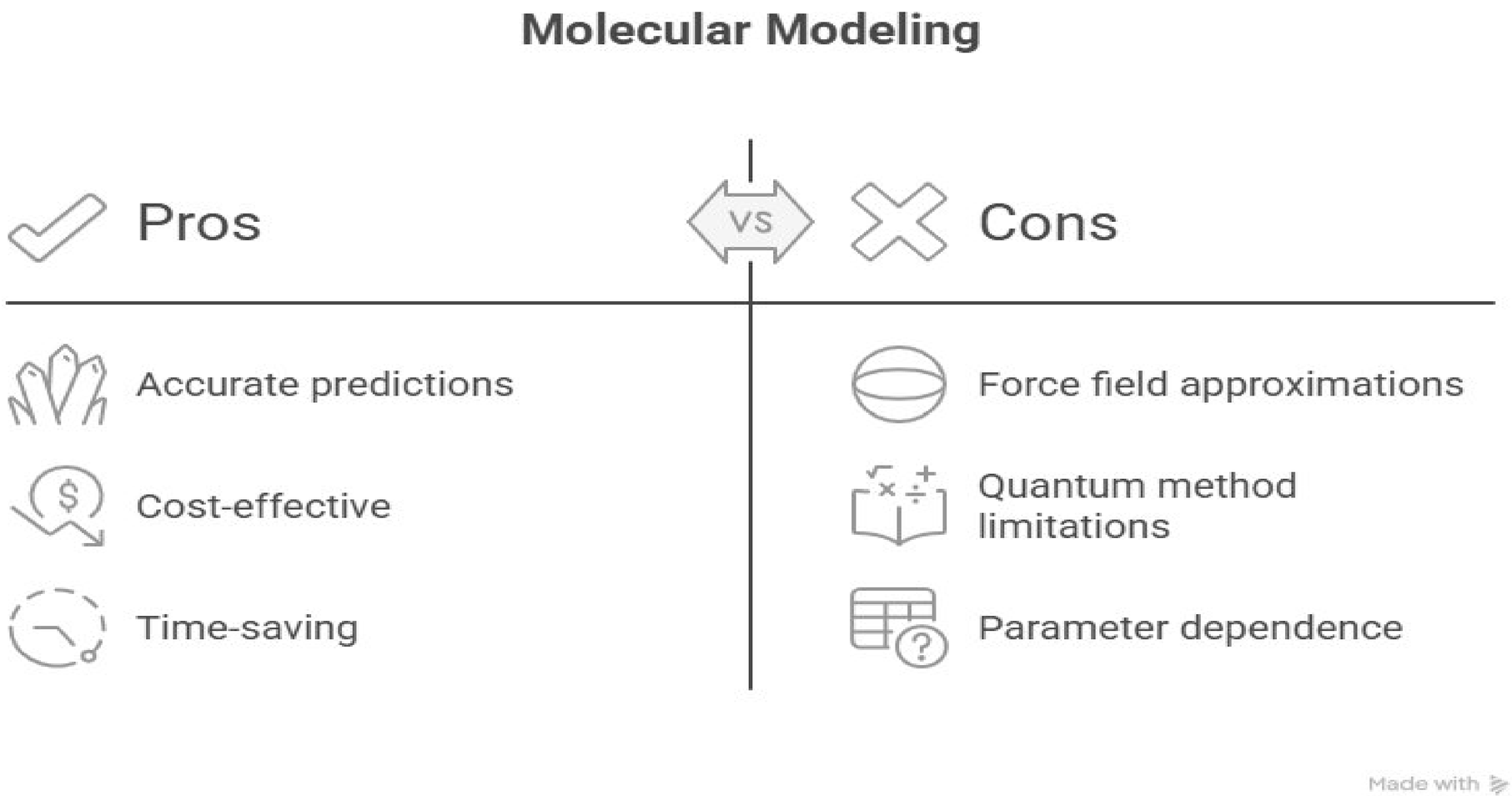
BENEFITS-PREDICTIVE POWER AND INSIGHT



BENEFITS-VISUALIZATION AND COMMUNICATION



WEAKNESS-ACCURACY AND APPROXIMATIONS



WEAKNESS-COST AND SCALABILITY

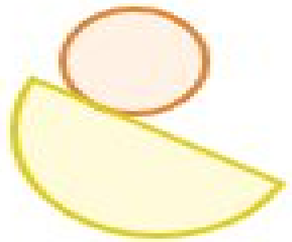
Molecular Modeling Challenges

Scalability Issues

Cost increases with atoms

High-Performance Computing

Requires supercomputers or clusters



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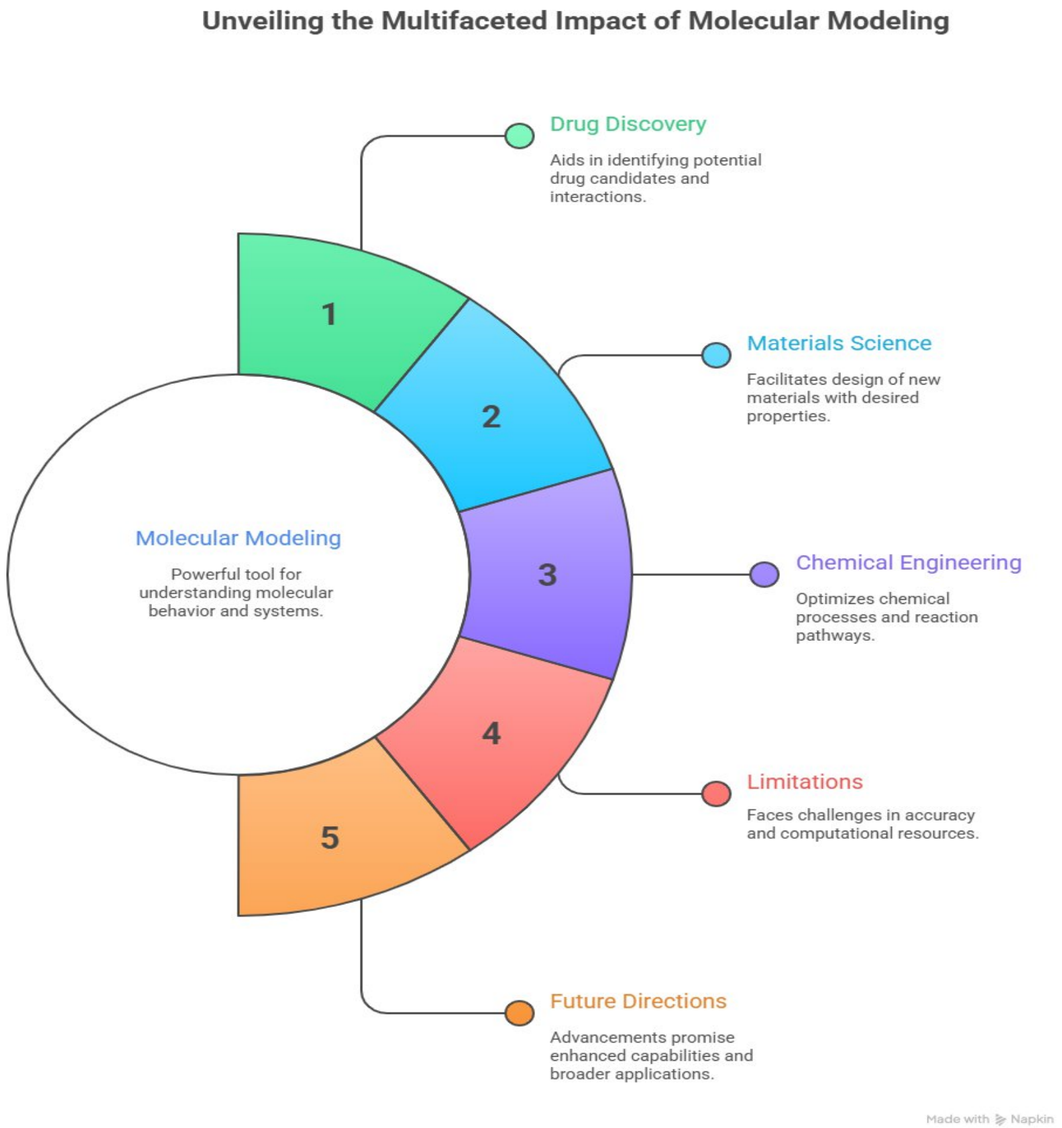
CONCLUSION


Unveiling the Multifaceted Impact of Molecular Modeling
Drug Discovery
Aids in identifying potential drug candidates and interactions.
Materials Science
Facilitates design of new materials with desired properties.
Chemical Engineering
Optimizes chemical processes and reaction pathways.
Limitations
Faces challenges in accuracy and computational resources.
Future Directions
Advancements promise enhanced capabilities and broader applications.
Molecular Modeling
Powerful tool for understanding molecular behavior and systems.
1
2
3
4
5
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ASSESMENTS

1] Molecular modeling is primarily used to:

a) Synthesize chemicals

b) Predict molecular behavior

c) Measure reaction temperature

d) Perform titrations

2]Which force field is commonly used in molecular mechanics?

a) Hartree–Fock

b) AMBER

c) DFT

d) MP2

3] Bond stretching in molecular mechanics is treated as:

a) Linear motion

b) Harmonic oscillation

c) Random motion

d) Quantum tunneling

4] Which software is used for molecular visualization?

a) Excel

b) PyMOL

c) SPSS

d) MATLAB

5] Molecular dynamics simulations study:

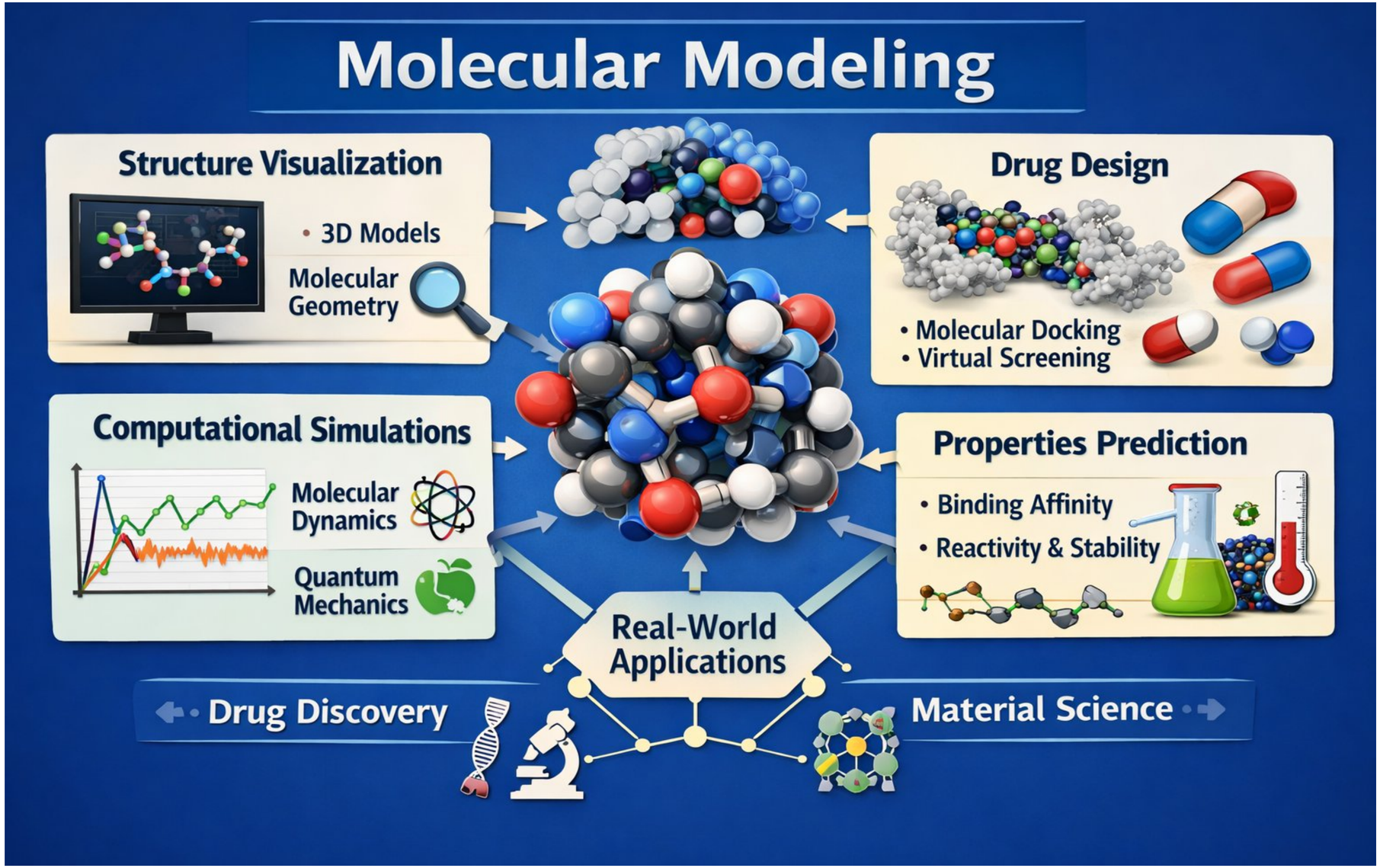
a) Static molecules

b) Reaction yield

c) Time-dependent molecular motion

d) pH changes

SUMMARY


Molecular Modeling
Structure Visualization
• 3D Models
Molecular Geometry
Drug Design
• Molecular Docking
• Virtual Screening
Computational Simulations
Molecular Dynamics
Quantum Mechanics
Properties Prediction
• Binding Affinity
• Reactivity & Stability
Real-World Applications
Drug Discovery
Material Science

REFERENCES

1]Leach, A. R. (2001). Molecular Modelling: Principles and Applications (2nd ed.). Pearson Education → Best core reference for molecular modeling fundamentals.

2]Jensen, F. (2017). Introduction to Computational Chemistry (3rd ed.). Wiley.→ Covers quantum mechanics, simulations, and modeling methods

3]Cramer, C. J. (2013). Essentials of Computational Chemistry: Theories and Models (2nd ed.). Wiley.

REFERENCES

4]Sliwoski, G., Kothiwale, S., Meiler, J., & Lowe, E. W. (2014).Computational methods in drug discovery. Pharmacological Reviews, 66(1), 334–395.→ Excellent for drug design & docking.

5]Karplus, M., & McCammon, J. A. (2002). Molecular dynamics simulations of biomolecules. Nature Structural Biology, 9(9), 646–652.

6]Kitchen, D. B., Decornez, H., Furr, J. R., & Bajorath, J. (2004). Docking and scoring in virtual screening for drug discovery. Nature Reviews Drug Discovery, 3, 935–949.


Thank You!