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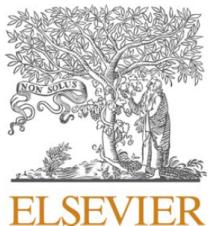


Hybrid Computational Algorithms for Molecular Structure Optimization and Global Minimum Search

Osvaldo Yáñez Osses, Ph.D.

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Noviembre - 2025



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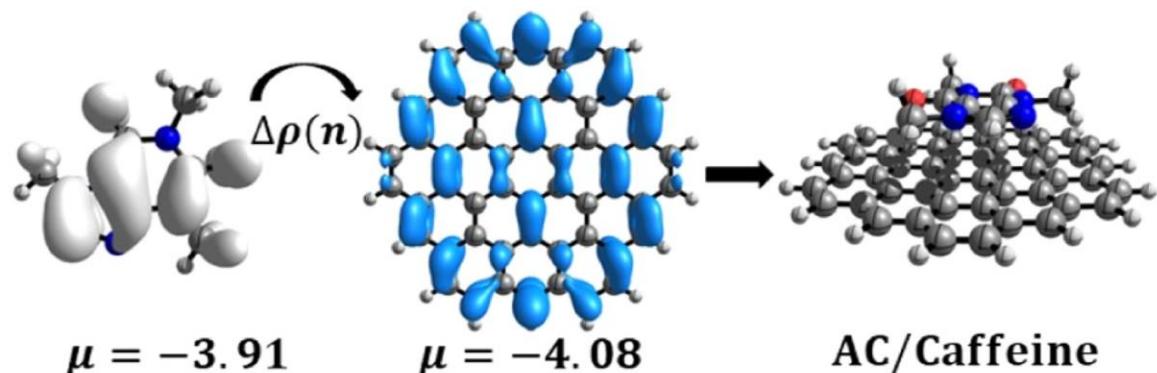
Journal of Environmental Chemical Engineering

journal homepage: www.elsevier.com/locate/jece

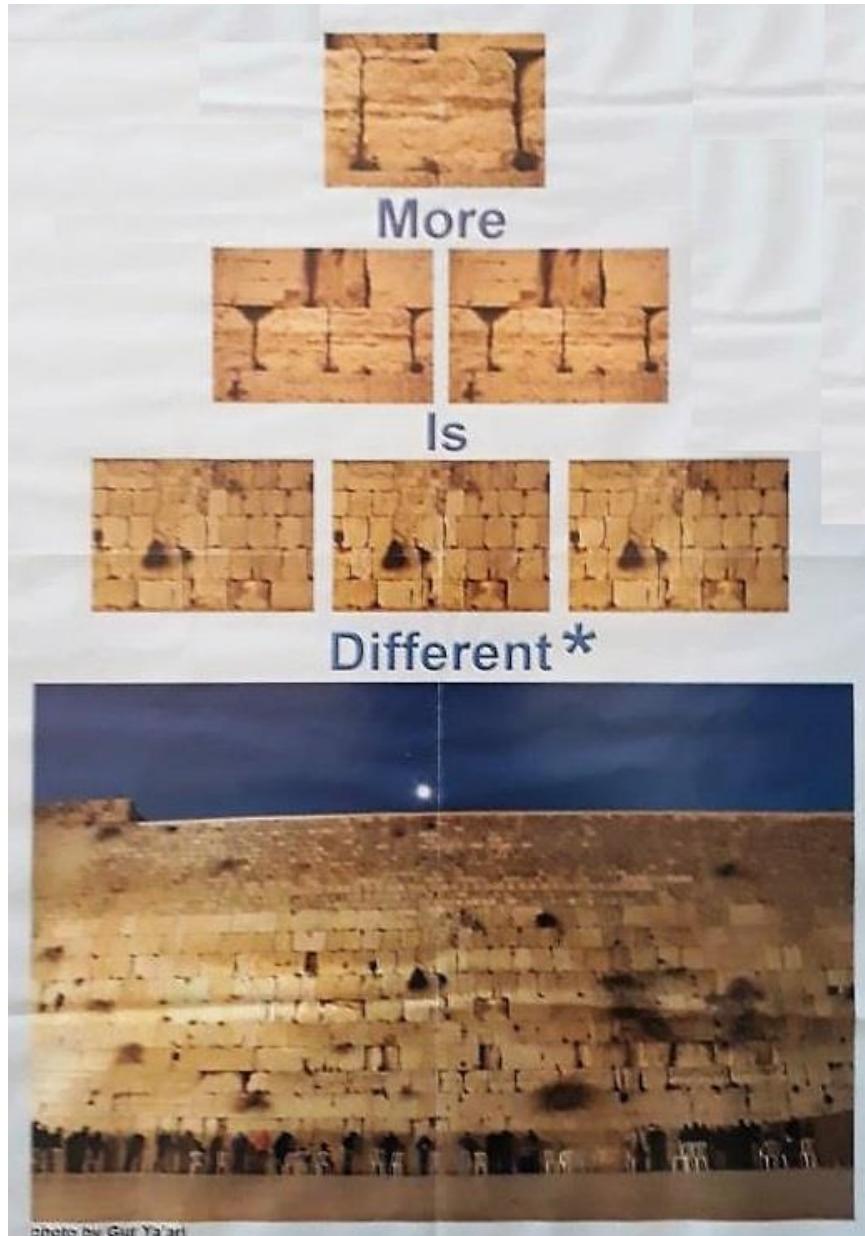


Exploring the adsorption of five emerging pollutants on activated carbon: A theoretical approach

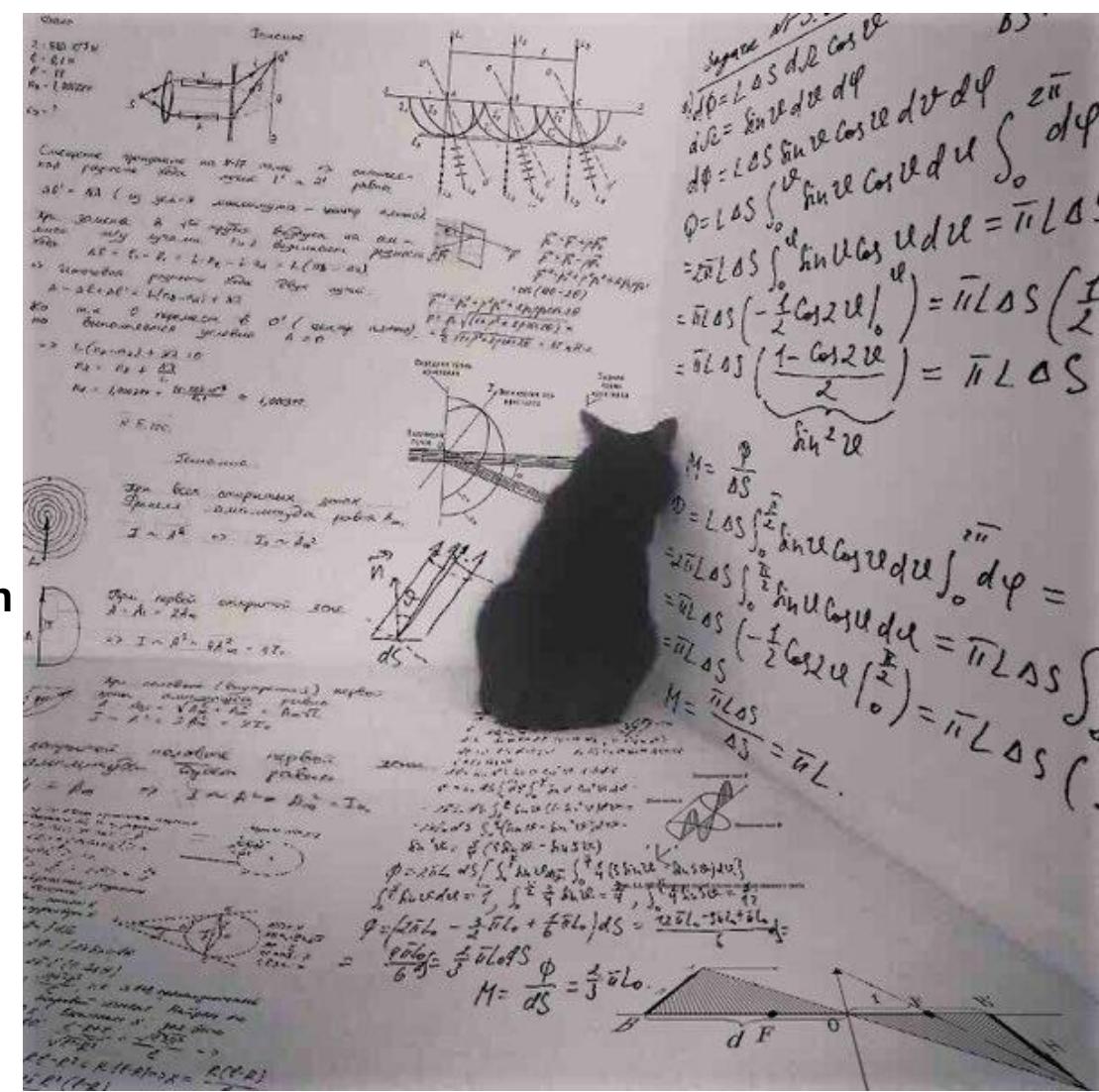
Lisdelys González-Rodríguez ^{a,b}, Osvaldo Yáñez ^b, Karel Mena- Ulecia ^{c,d}, Yoan Hidalgo-Rosa ^{e,f}, Ximena García- Carmona ^g, Claudia Ulloa- Tesser ^{h,*}

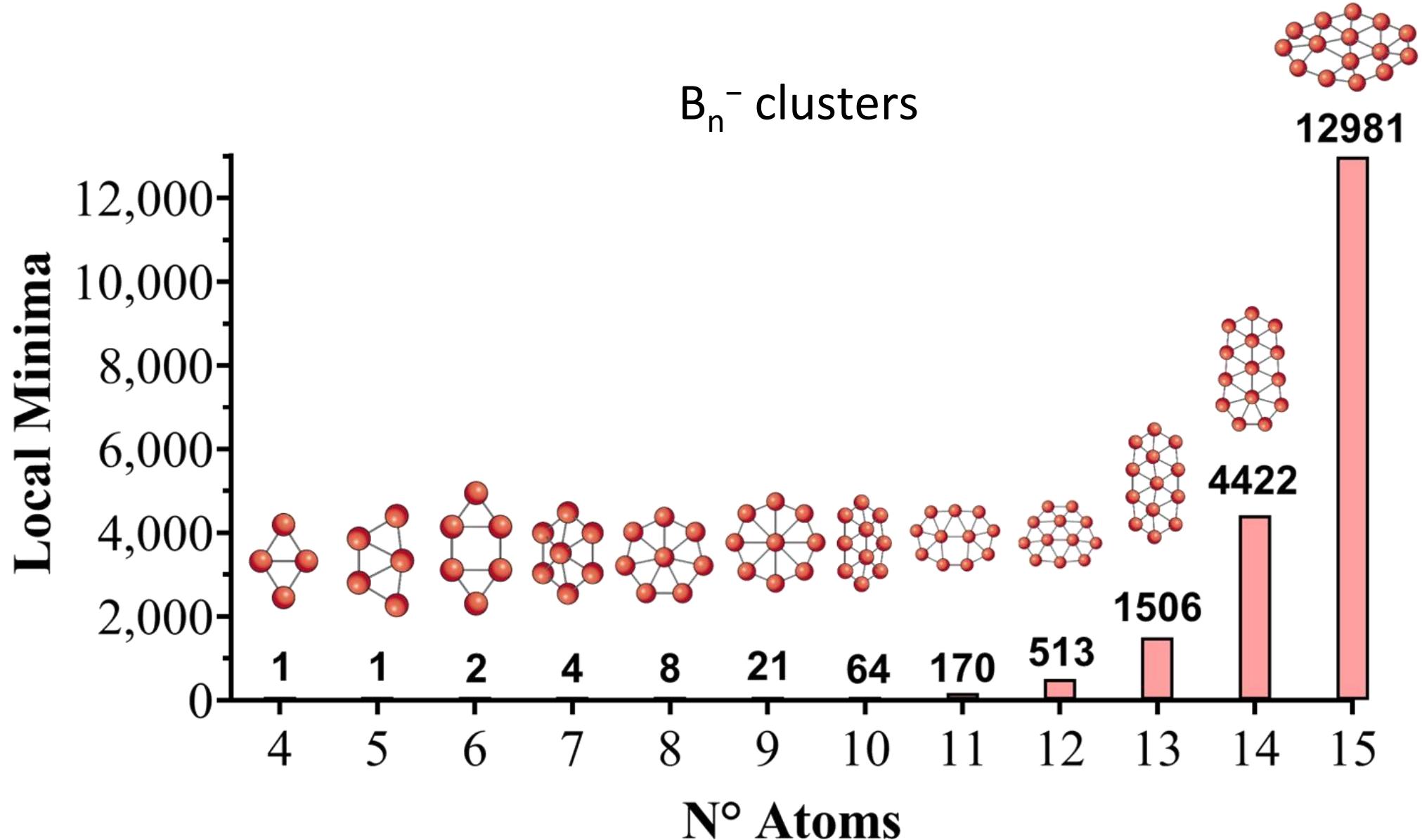


More is Different

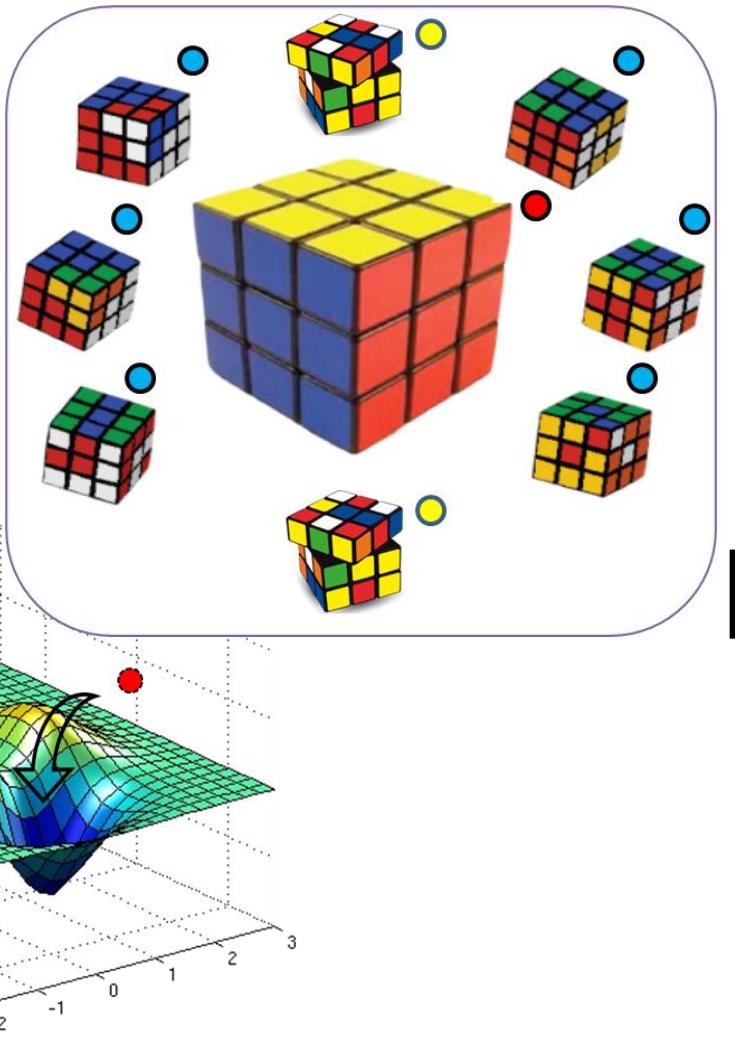


Philip Warren Anderson





Paradoxes



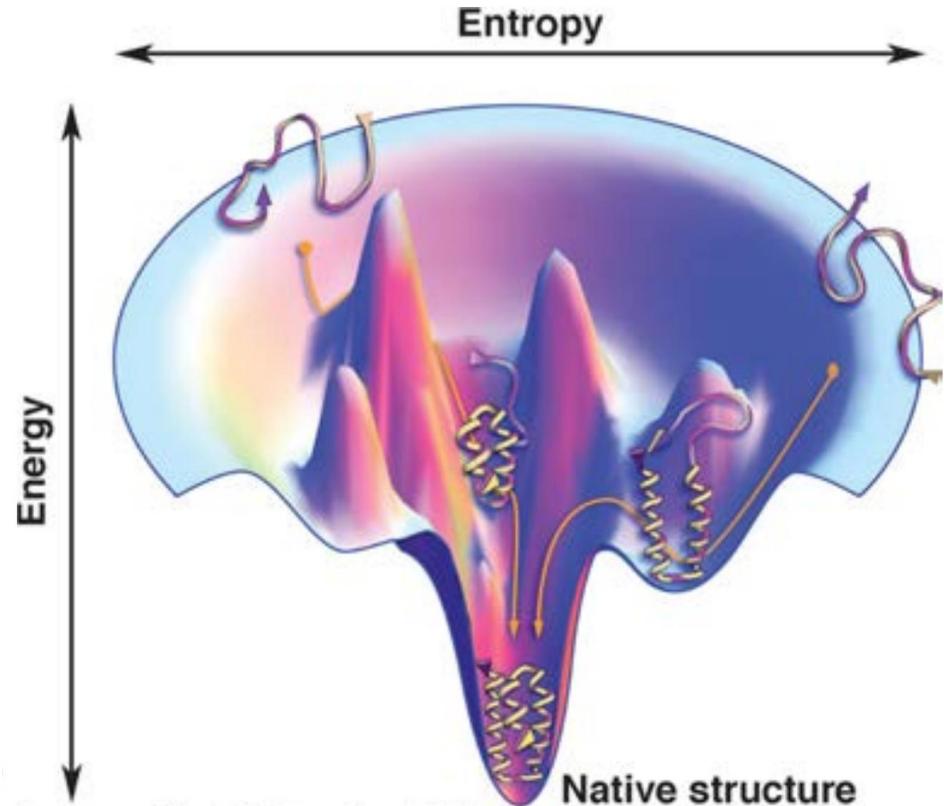
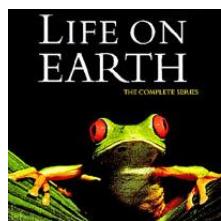
$$N_{cfg} = 4.33 \times 10^{19}$$

$$1.37 \times 10^{12} \text{ años}$$

$$1.37 \times 10^{10} \text{ años}$$



$$3.5 \times 10^9 \text{ años}$$

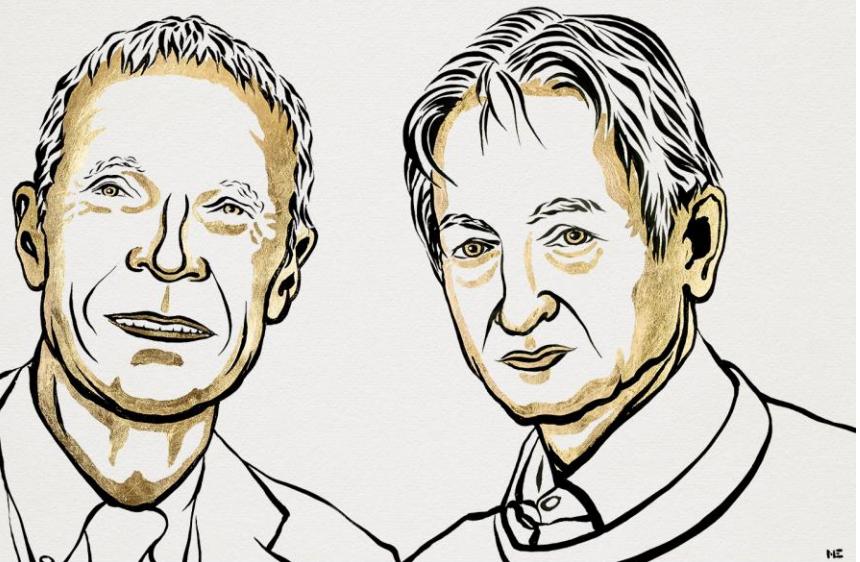


$$N_{cfg} = 5 \times 10^{47}$$

$$3.20 \times 10^{98} \text{ años}$$

THE NOBEL PRIZE IN PHYSICS 2024

Illustrations: Niklas Elmehed

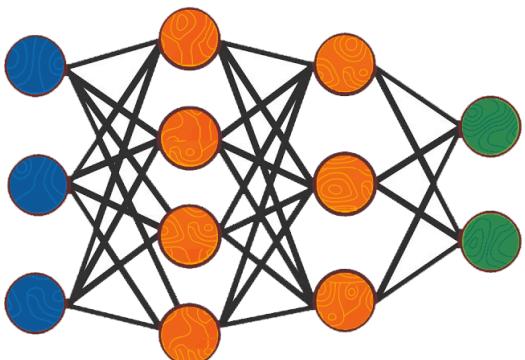


John J. Hopfield

Geoffrey E. Hinton

"for foundational discoveries and inventions
that enable machine learning
with artificial neural networks"

THE ROYAL SWEDISH ACADEMY OF SCIENCES



Illustrations: Niklas Elmehed

THE NOBEL PRIZE IN CHEMISTRY 2024



**David
Baker**

**Demis
Hassabis**

**John M.
Jumper**

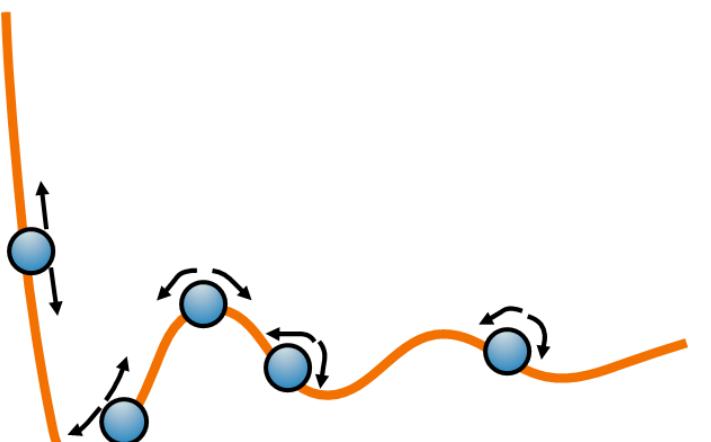
"for computational
protein design"

"for protein structure prediction"

THE ROYAL SWEDISH ACADEMY OF SCIENCES

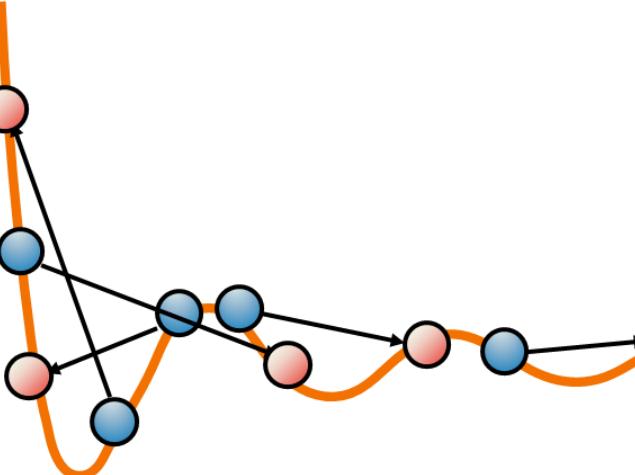
Deterministic algorithm

- Gradient Descent/Ascent
- Molecular dynamics
- Whole/non-linear programming



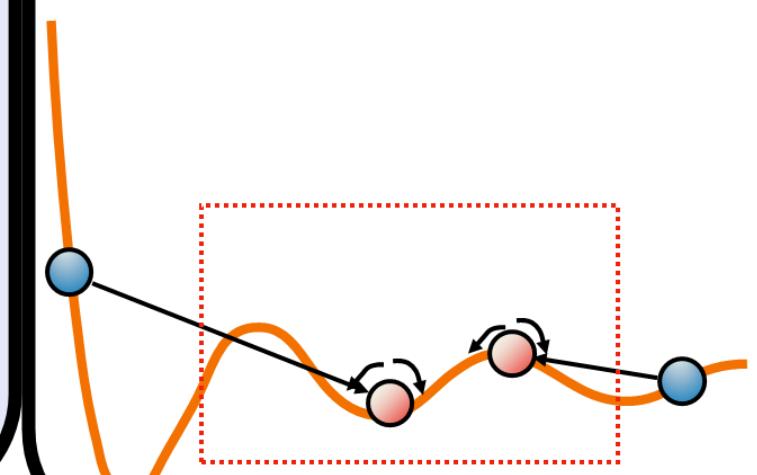
Stochastic algorithm

- Simulated Annealing
- Evolutionary Algorithms
- Kick Algorithm
- Pure Random Search



Hybrid algorithm

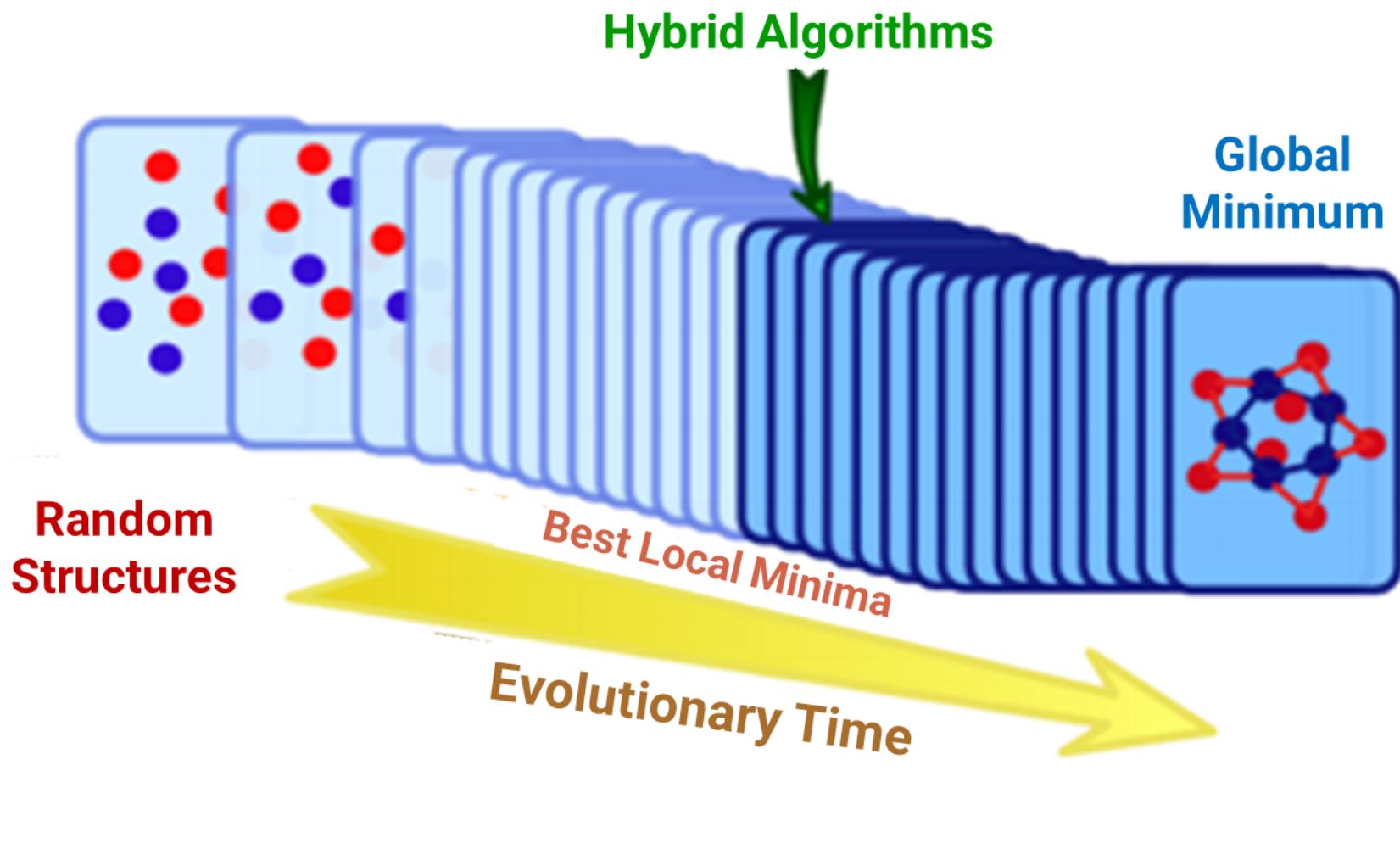
- Local + Local
- Global + Local (*Memetic*)
- Global + Global

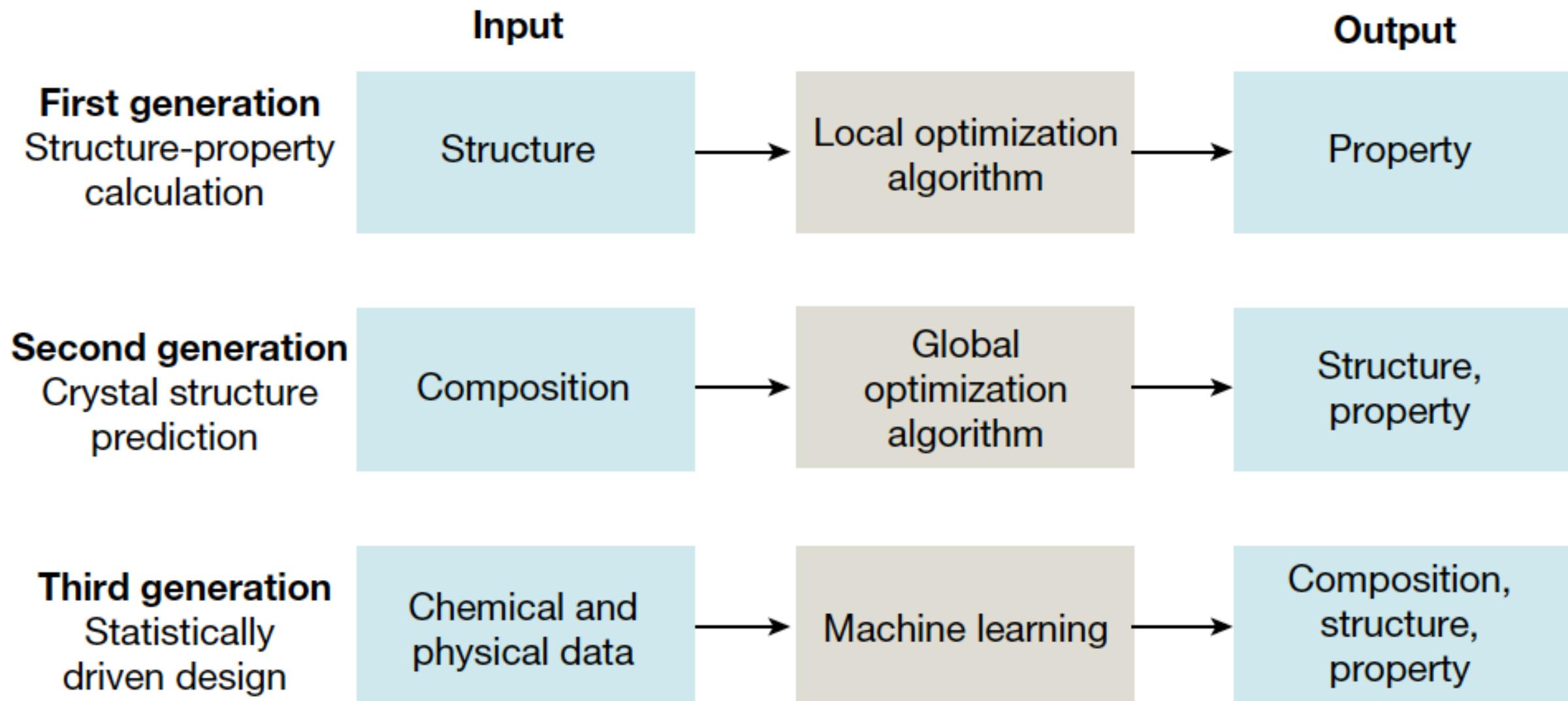


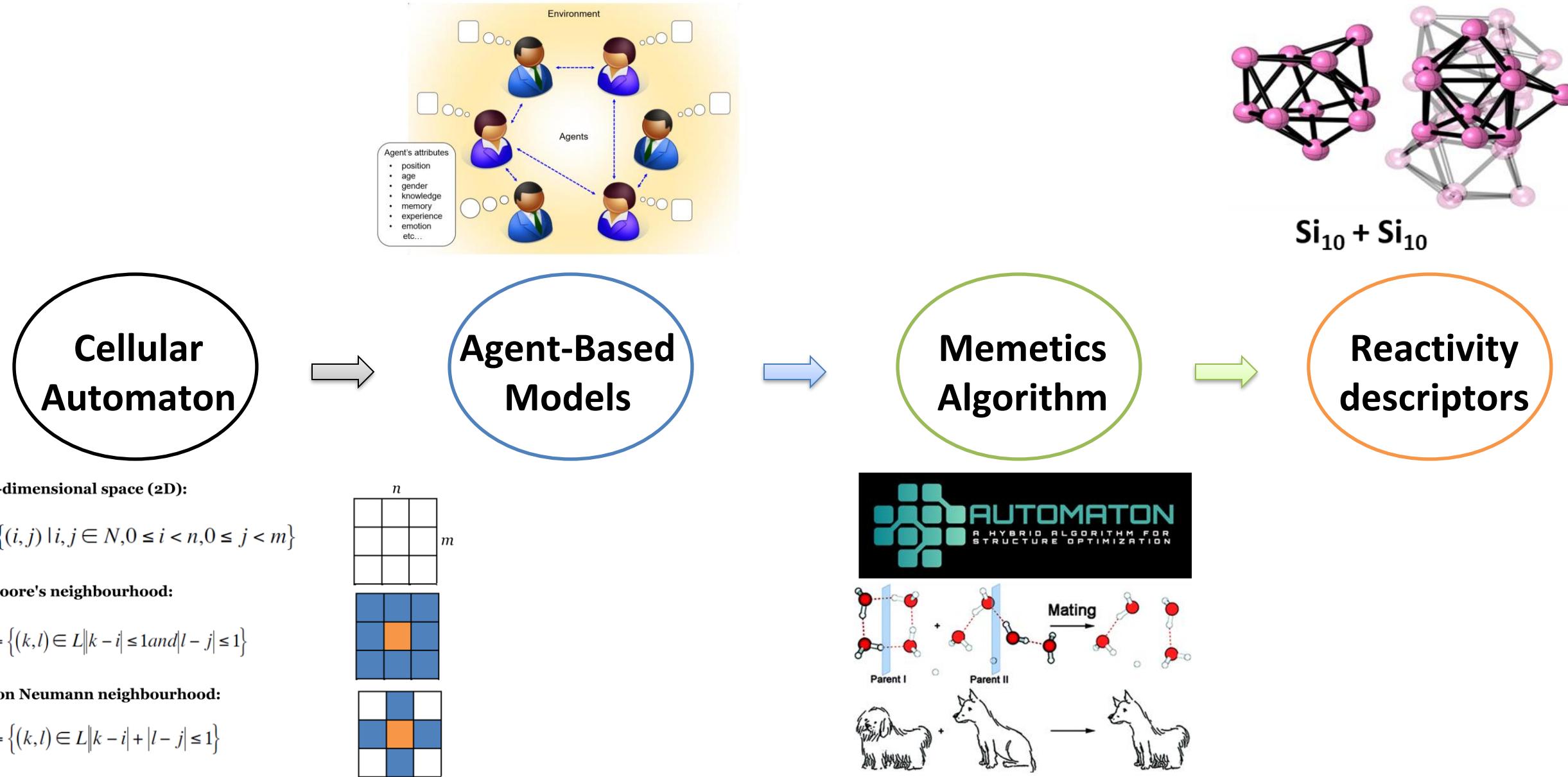


Richard Dawkins. **The Selfish Gene** (1976)

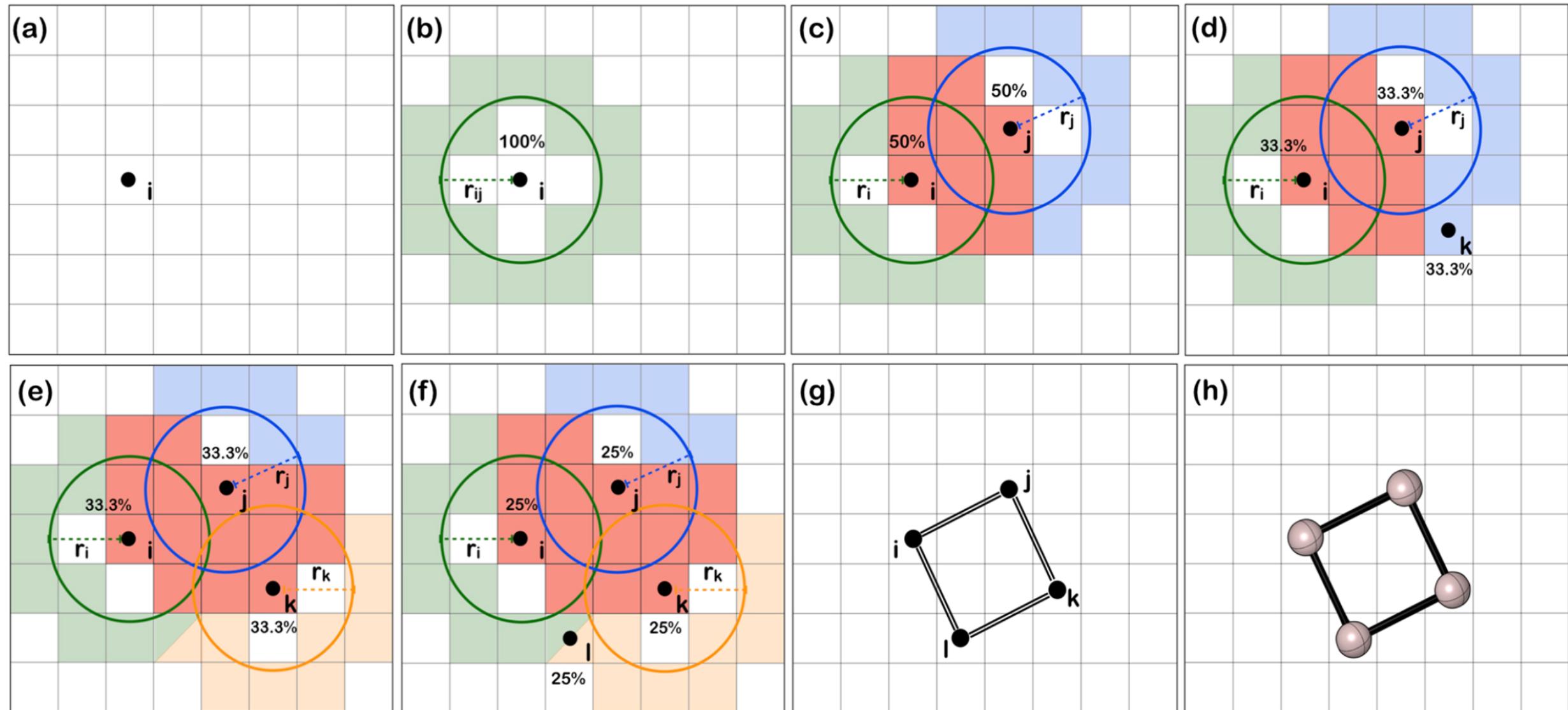
Memes are patterns of information, ideas, behaviours, or symbols that are replicated and spread throughout human culture through imitation, adaptation, and natural selection.







Scheme 1. Representation of the Cell Selection Procedure for the Construction of a Four-Atom Cluster^a



Deterministic ABM (Benzene)

Estructura molecular — paso 1

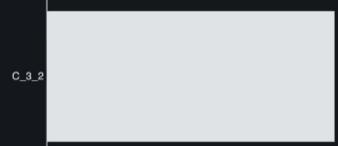


MAS Centralizado



Métricas (paso 1)
Átomos: 1
Enlaces: 0
Avance estructural: 0%
Saturación promedio: 0.00
% átomos saturados: 0%
Componentes conectados: 0
Enlaces por tipo:

Valencia actual vs esperada



Avance estructural



Componentes conectados

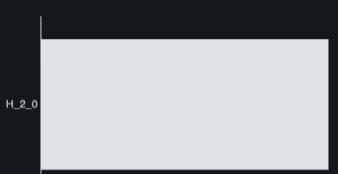


MAS Semidescentralizado



Métricas (paso 1)
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Enlaces: 0
Avance estructural: 0%
Saturación promedio: 0.00
% átomos saturados: 0%
Componentes conectados: 0
Enlaces por tipo:

Valencia actual vs esperada



Avance estructural



Componentes conectados

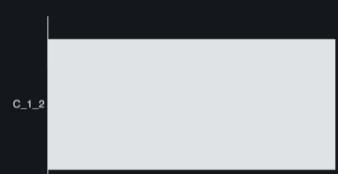


MAS Distribuido



Métricas (paso 1)
Átomos: 1
Enlaces: 0
Avance estructural: 0%
Saturación promedio: 0.00
% átomos saturados: 0%
Componentes conectados: 0
Enlaces por tipo:

Valencia actual vs esperada



Avance estructural



Componentes conectados



Stochastic ABM (Benzene)

Estructura molecular — paso 1



MAS Centralizado



MAS Semidescentralizado



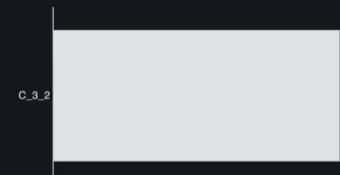
MAS Distribuido



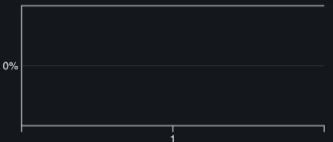
Métricas (paso 1)

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Enlaces por tipo:

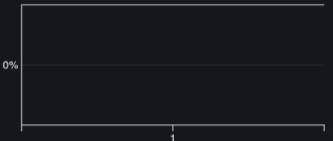
Valencia actual vs esperada



Avance estructural



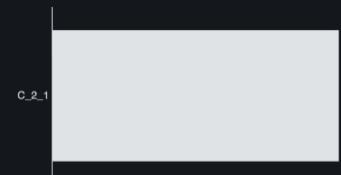
Componentes conectados



Métricas (paso 1)

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Componentes conectados: 0
Enlaces por tipo:

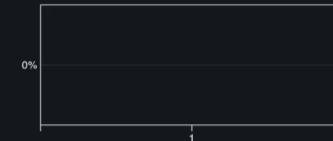
Valencia actual vs esperada



Avance estructural



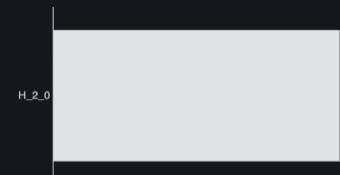
Componentes conectados



Métricas (paso 1)

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% átomos saturados: 0%
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Enlaces por tipo:

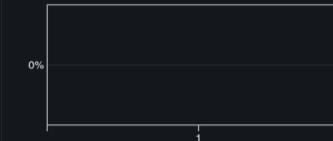
Valencia actual vs esperada

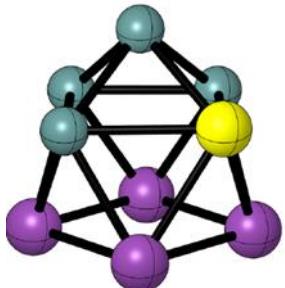


Avance estructural

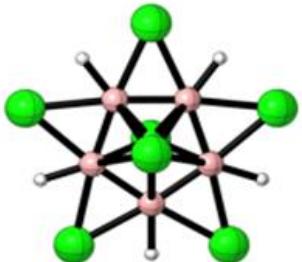


Componentes conectados

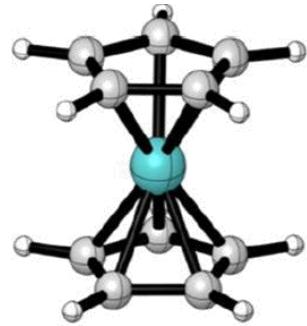




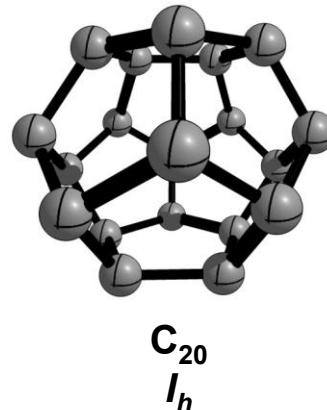
SnGe_4Bi_4
 C_s



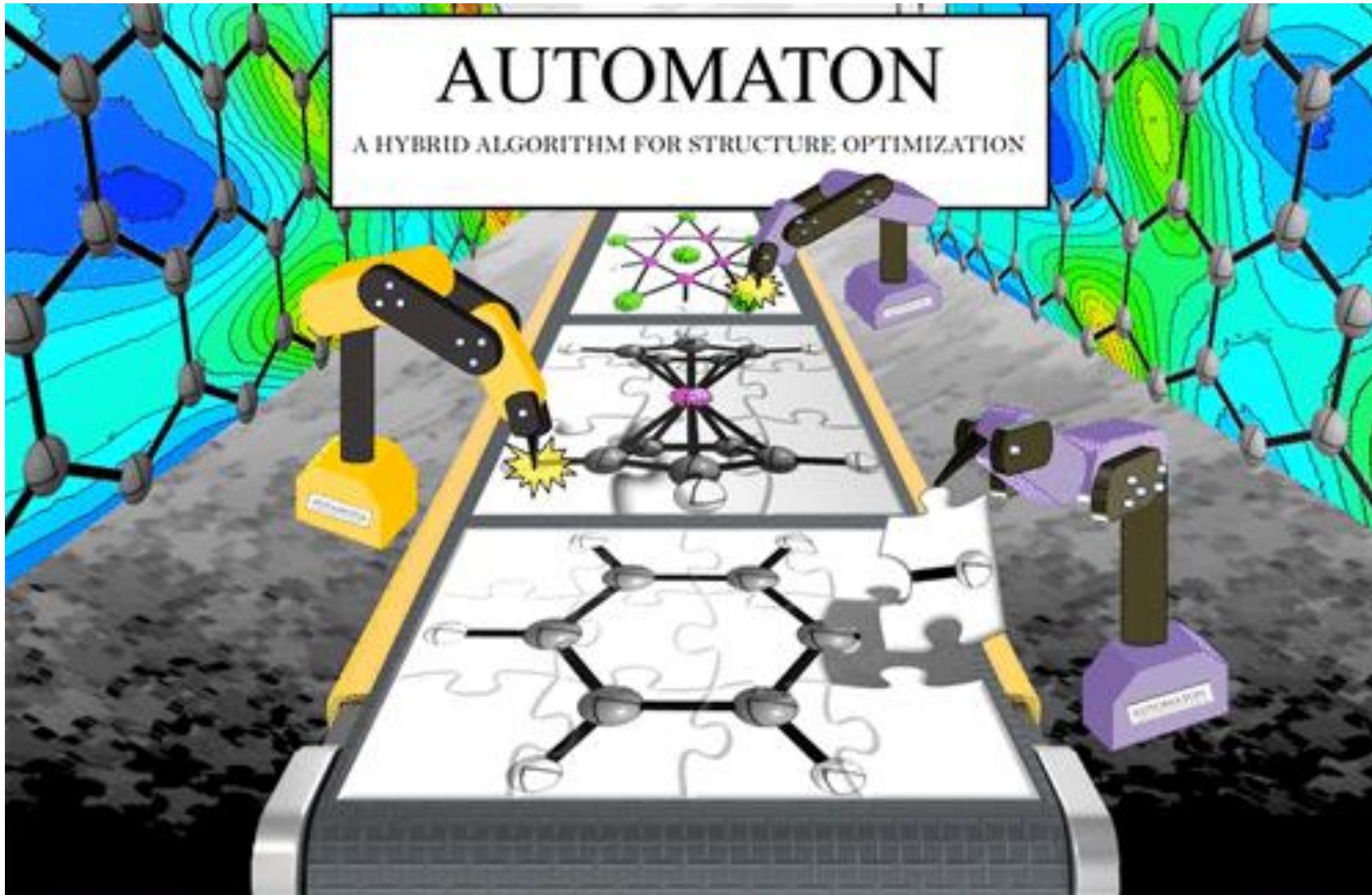
$\text{Li}_7(\text{BH})_5^+$
 D_{5h}



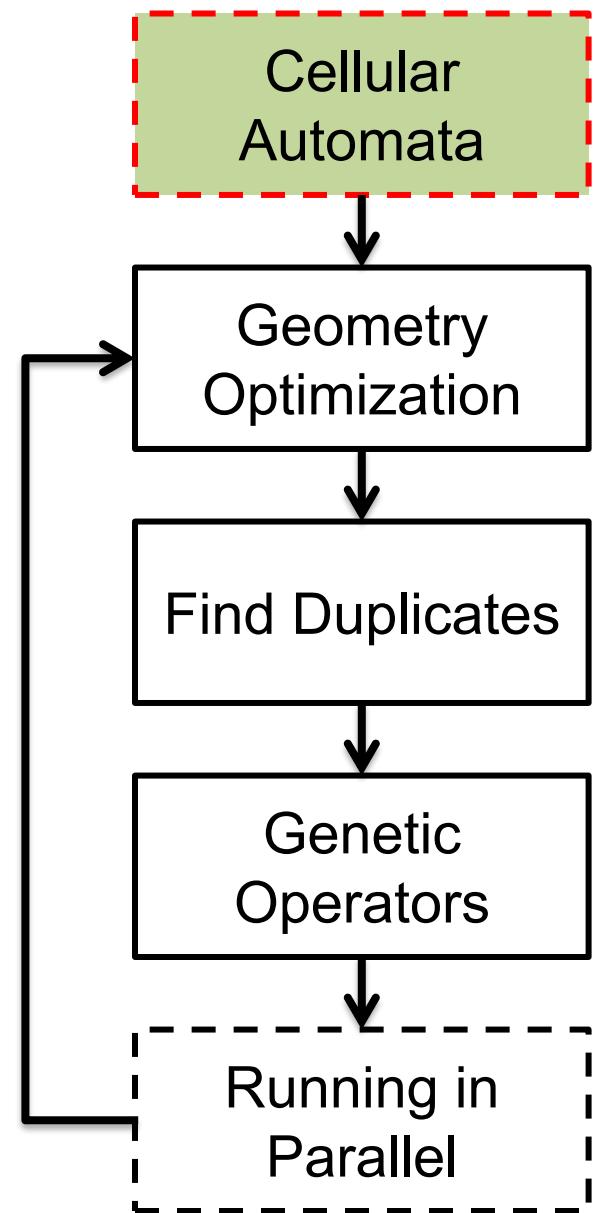
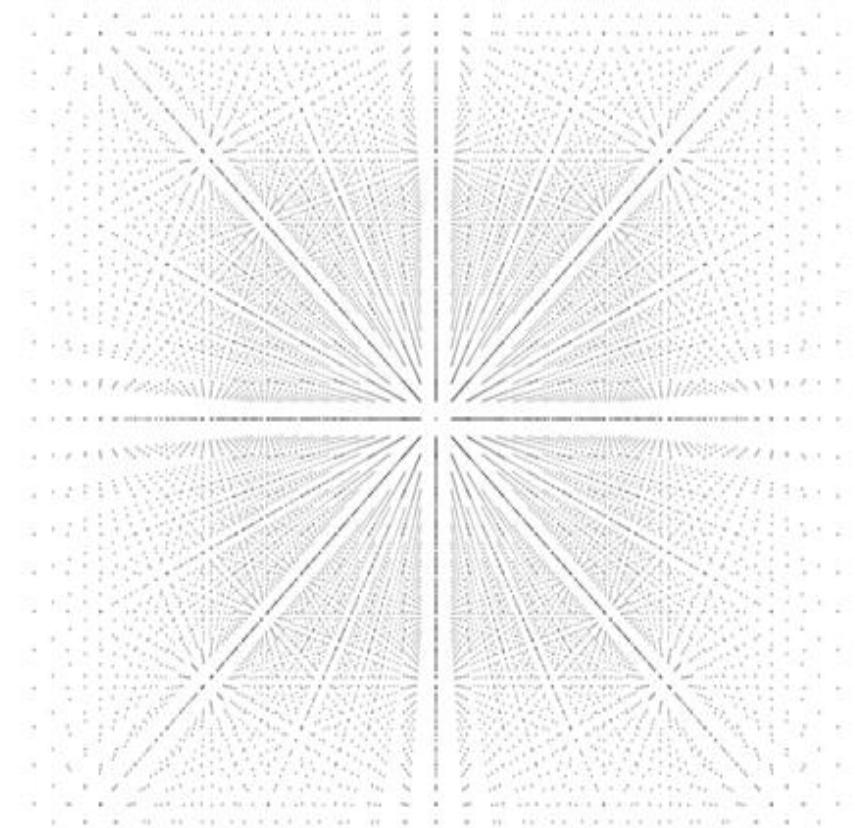
$\text{Fe}(\text{C}_5\text{H}_5)_2$
 D_{5h}

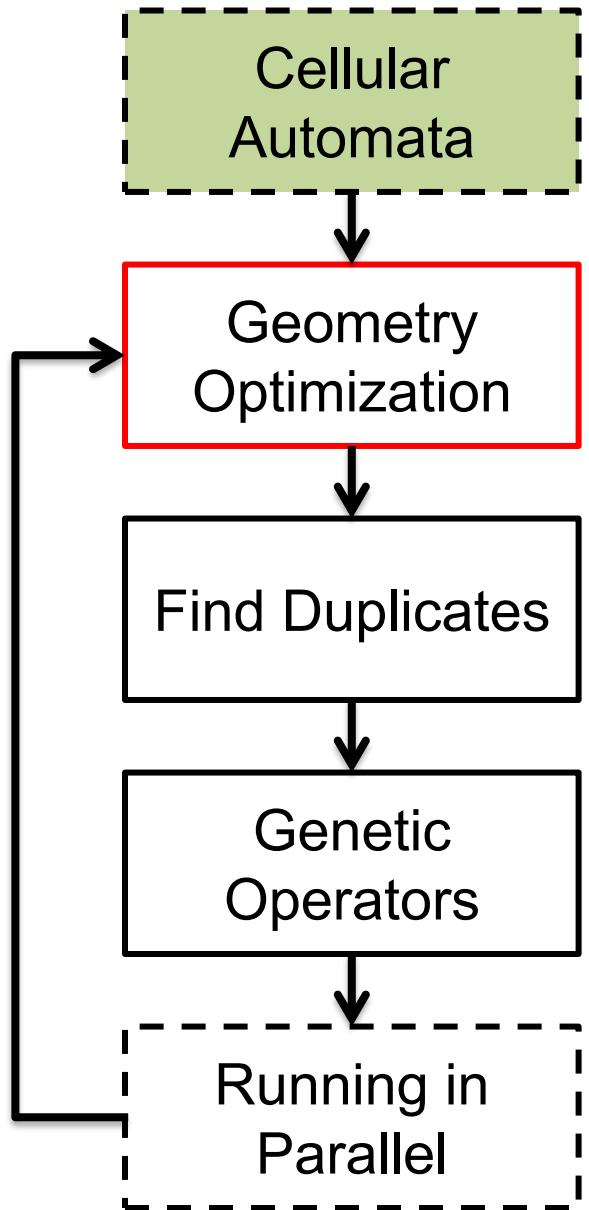
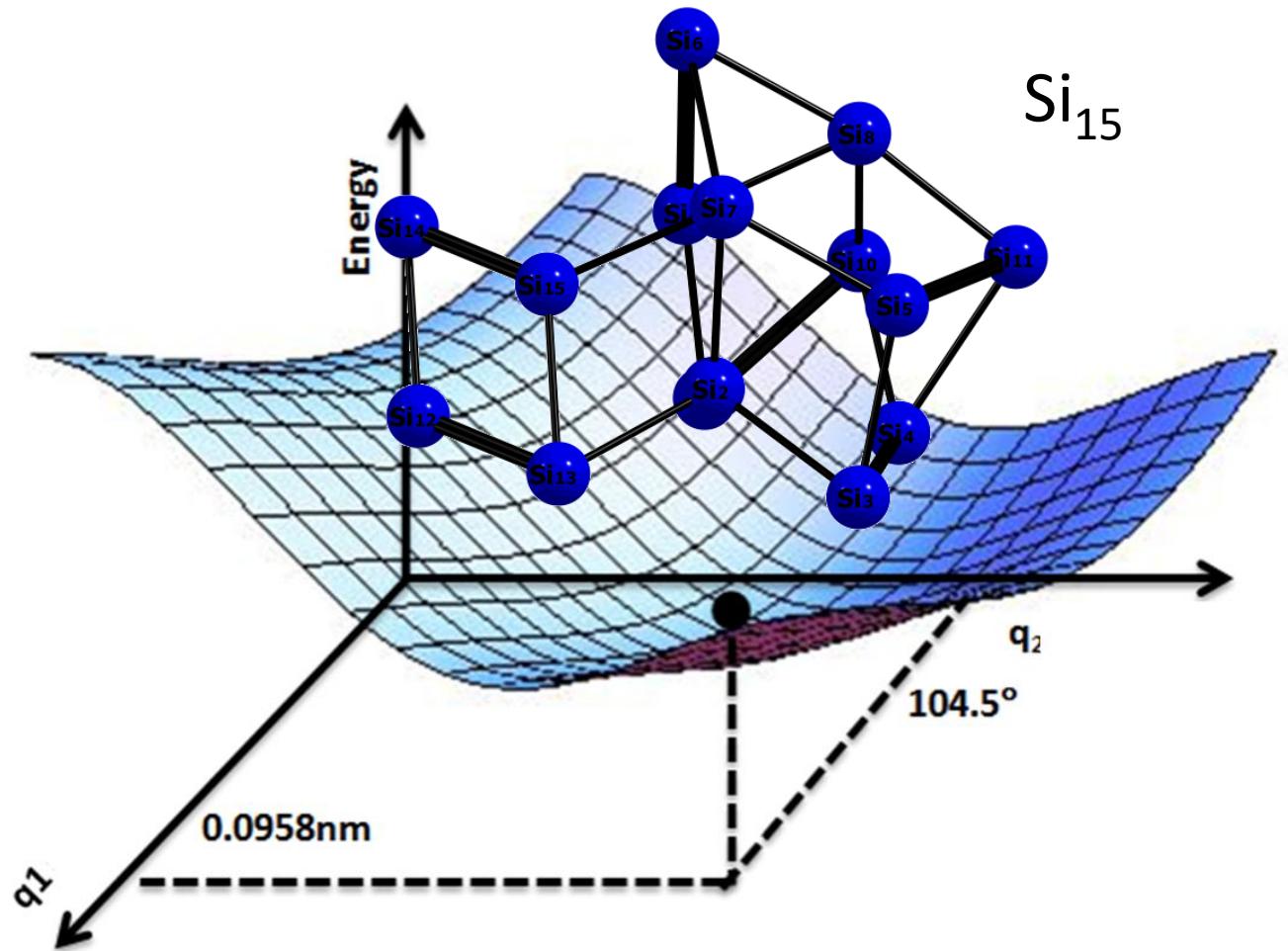


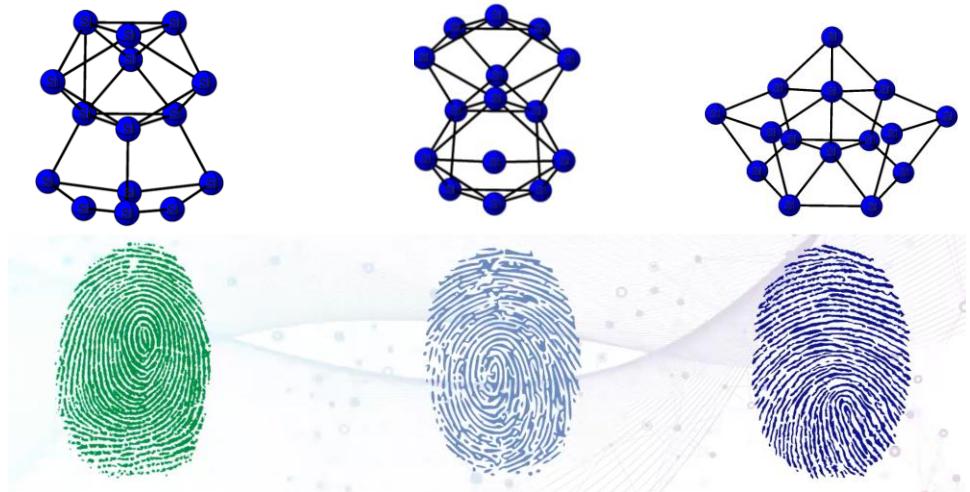
C_{20}
 I_h



AUTOMATON: A Program That Combines a Probabilistic Cellular Automata and a Genetic Algorithm for Global Minimum Search of Clusters and Molecules





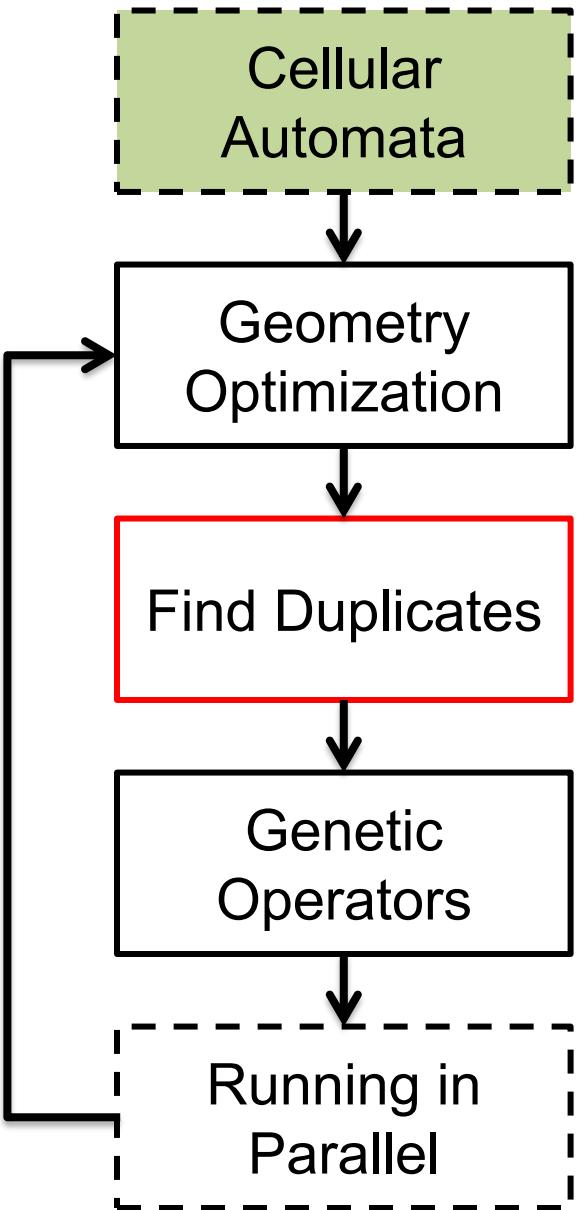


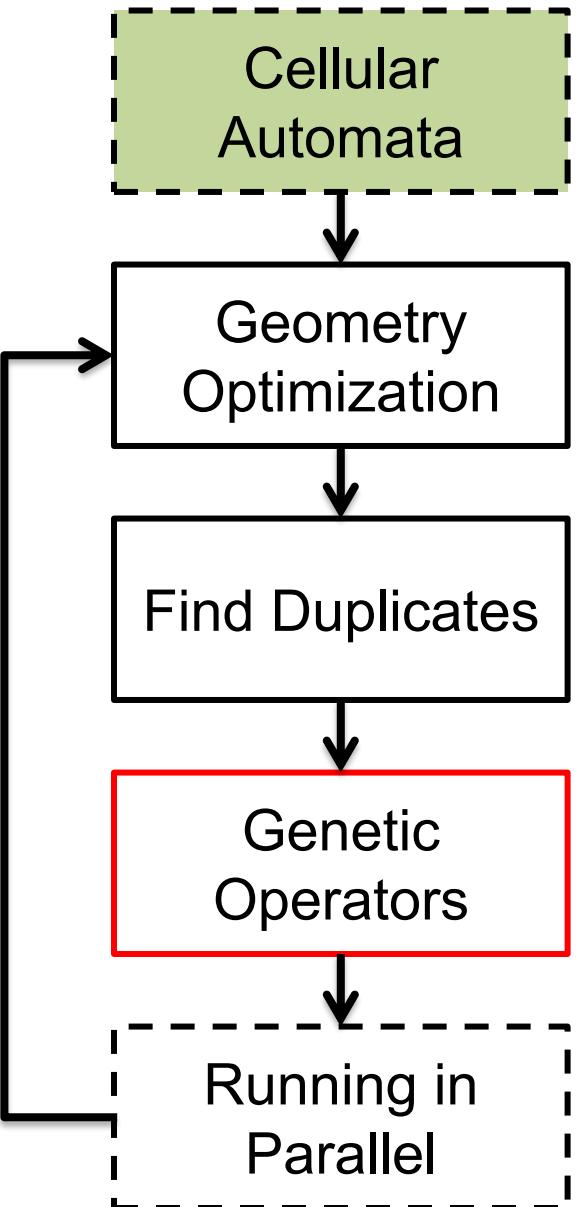
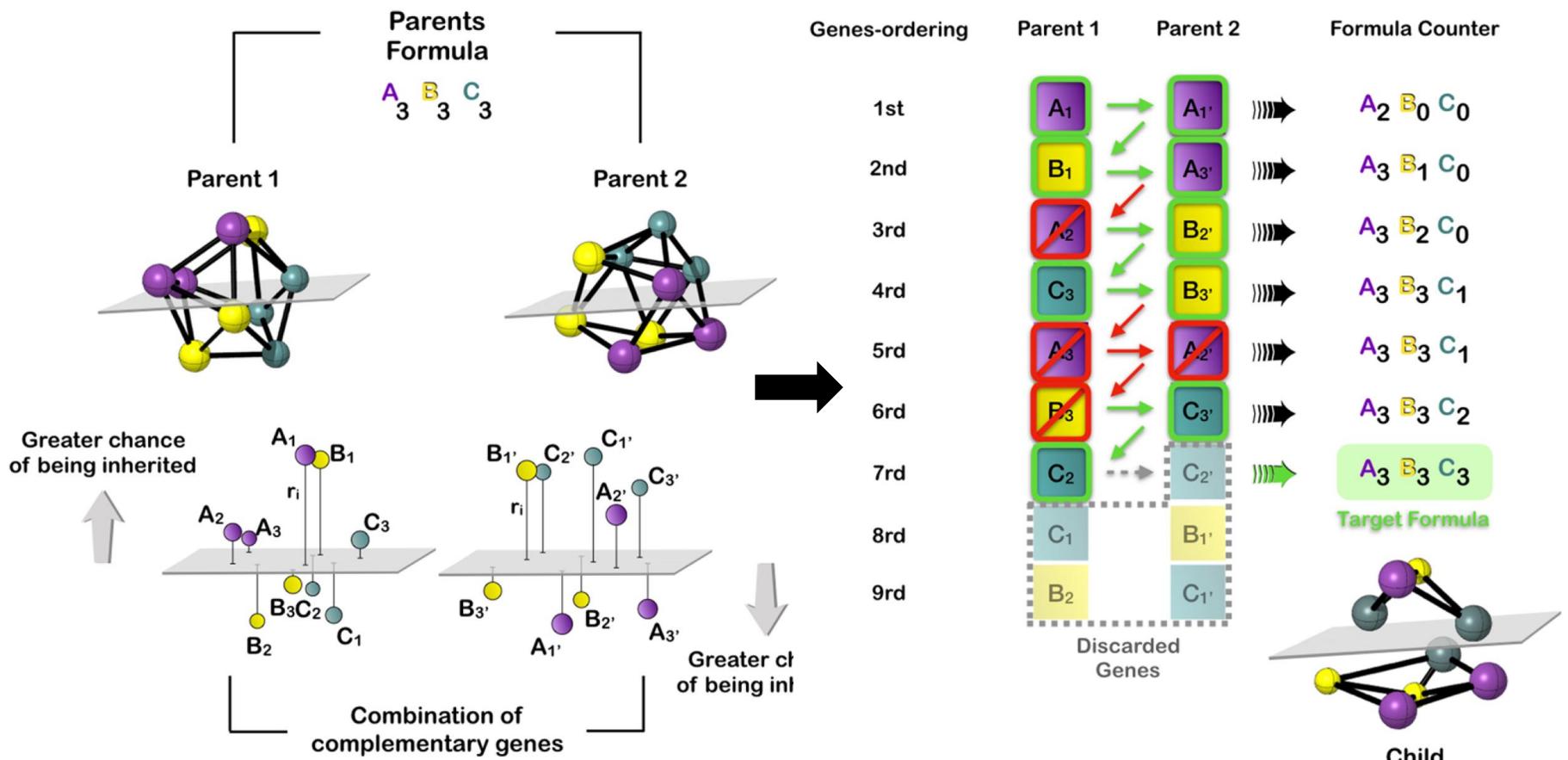
Distances

$$d^\tau(\alpha, \beta) = \left[\frac{2}{N(N-1)} \sum_{n=1}^{\frac{N(N-1)}{2}} \left(\frac{d_n^{(\alpha)}}{D_{ave}^{(\alpha)}} - \frac{d_n^{(\beta)}}{D_{ave}^{(\beta)}} \right)^2 \right]^{1/2}$$

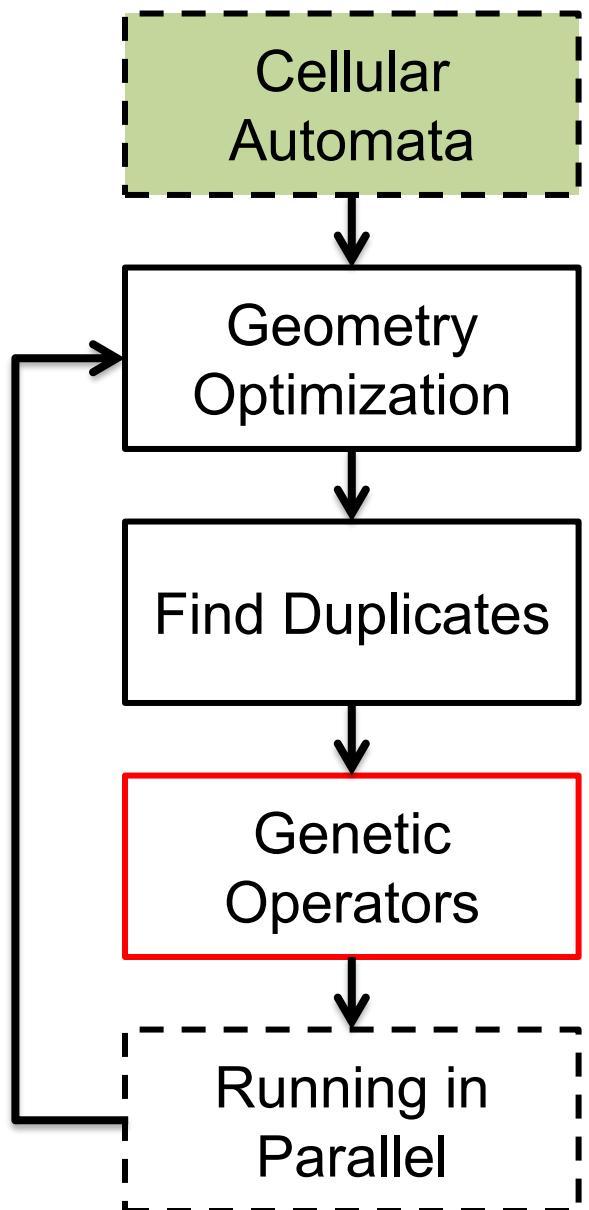
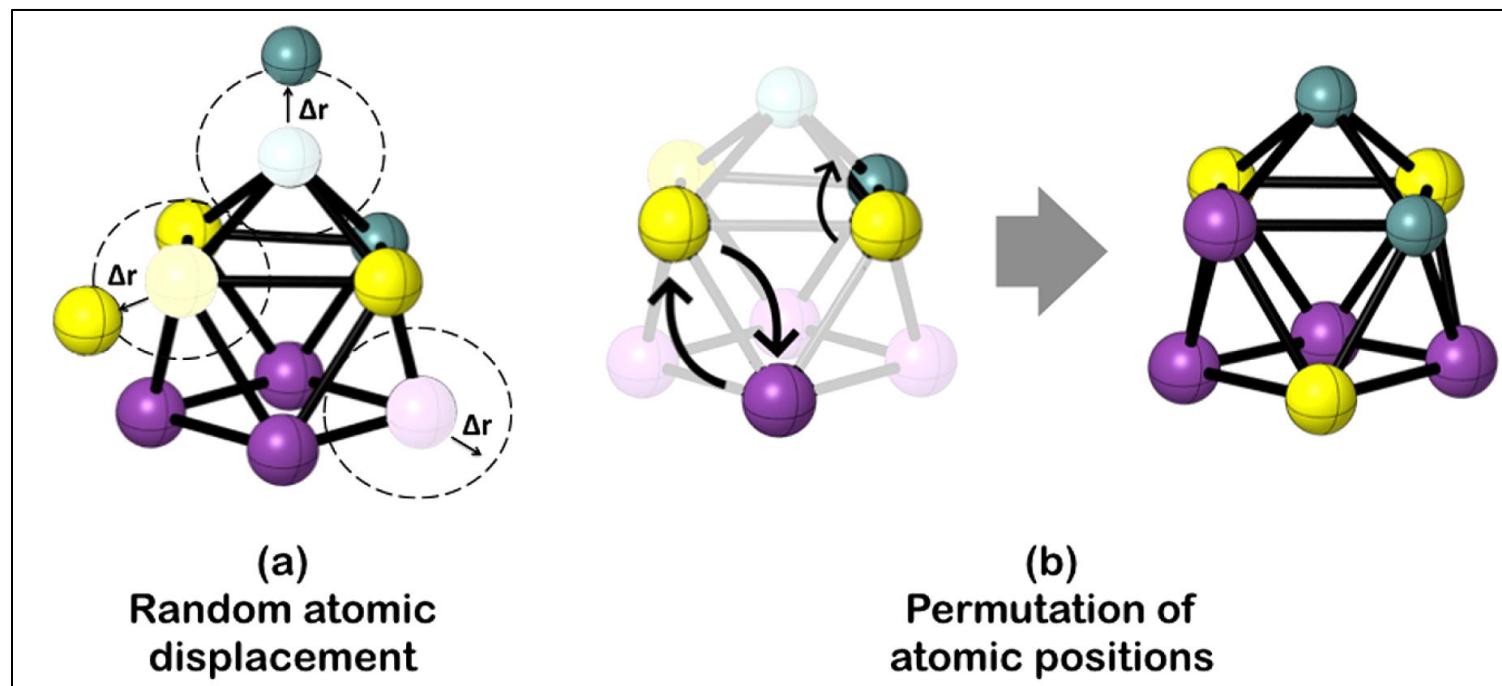
Charge

$$q^r(\alpha, \beta) = \left[\frac{2}{N(N-1)} \sum_{n=1}^{N(N-1)} \left(\frac{q_n^{(\alpha)}}{Q_{ave}^{(\alpha)}} - \frac{q_n^{(\beta)}}{Q_{ave}^{(\beta)}} \right)^2 \right]^{1/2}$$

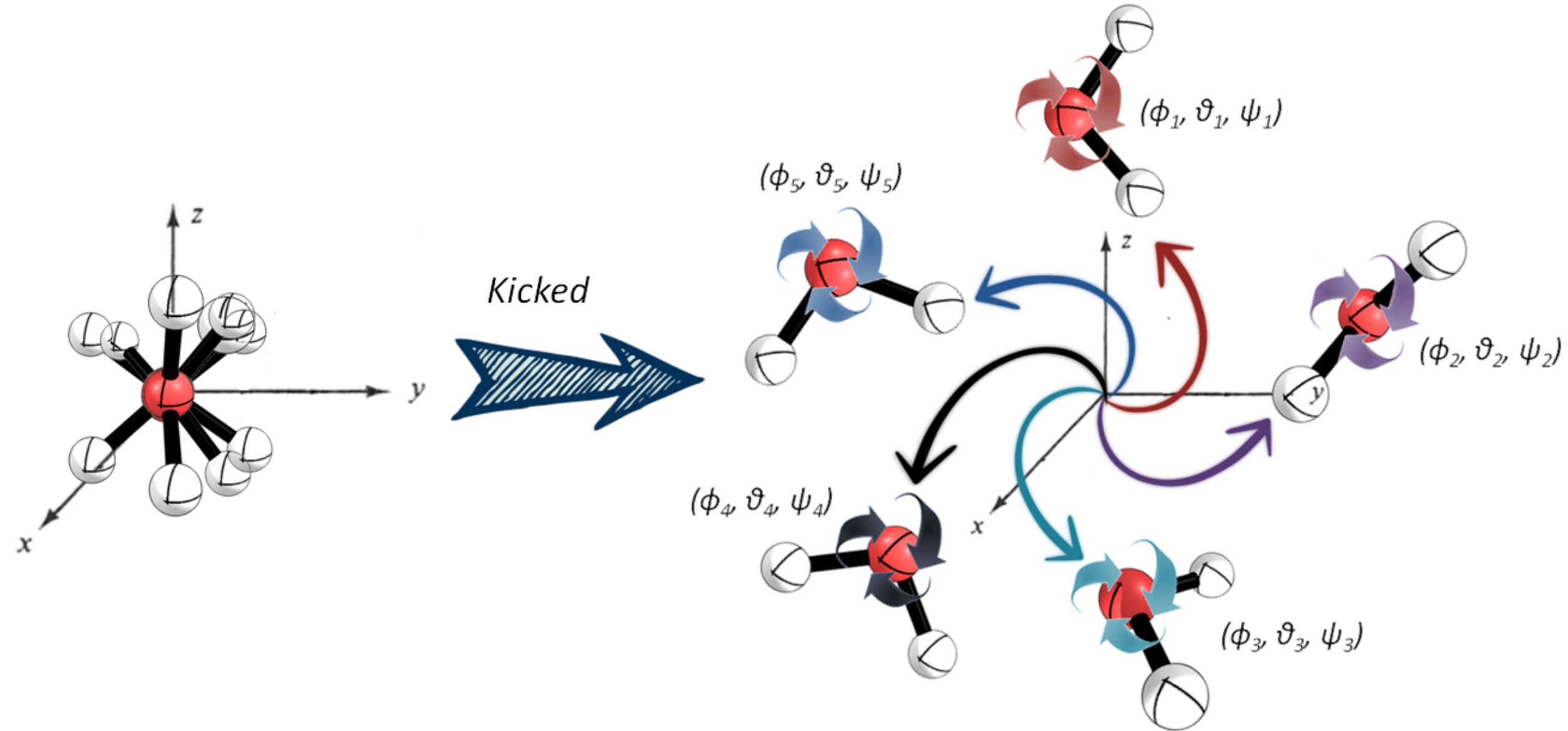




Representation of the Mutation Operation

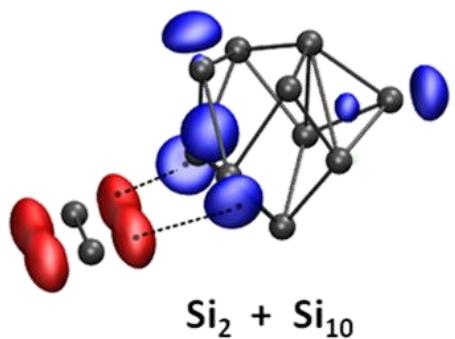


Stochastic Kick Algorithm



Fukui function

$$f(r) = \left(\frac{\delta\mu(r)}{\delta v(r)} \right)_N = \left(\frac{\partial\rho(r)}{\partial N} \right)_{v(r)}$$



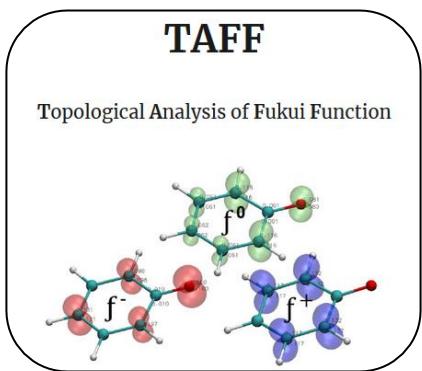
Topological analysis



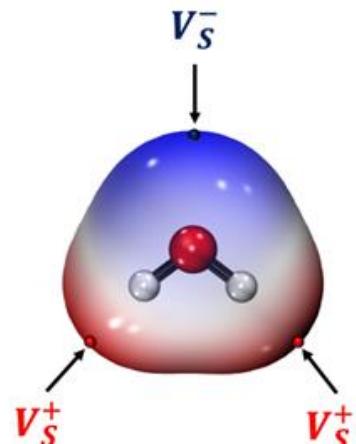
$$Jf_{AB} = \sum_{k=1}^{m'} \sum_{k'=1}^m \frac{f_{A,k}^+ f_{B,k'}^-}{r_{kk'}}$$

Electrostatic potential

$$V_{total}(r) = V_{Nuc}(r) + V_{Elec}(r) = \sum_A \frac{Z}{r} - \int \frac{\rho(r')}{|r - r'|} dr'$$



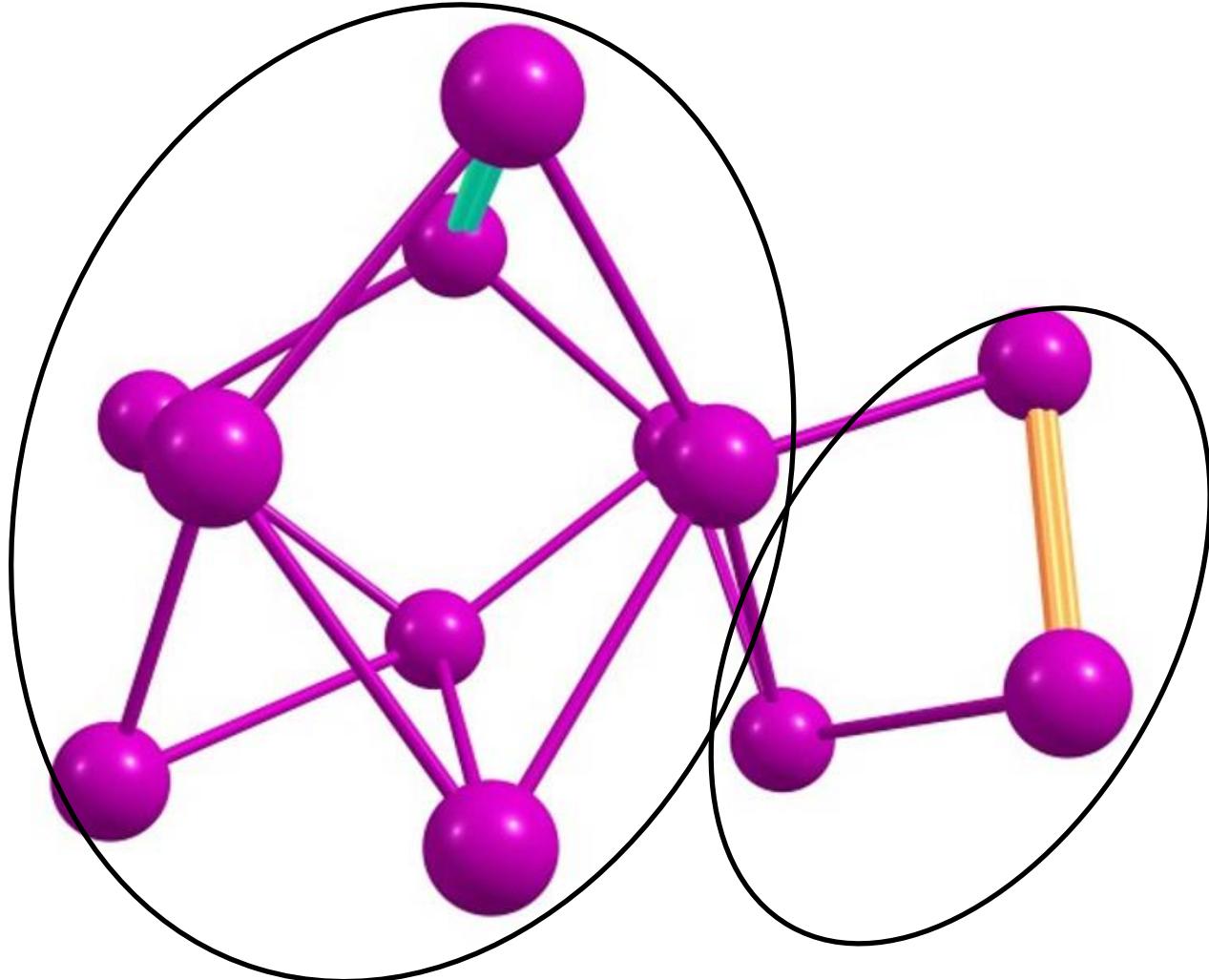
Koopmans and Finite Differences

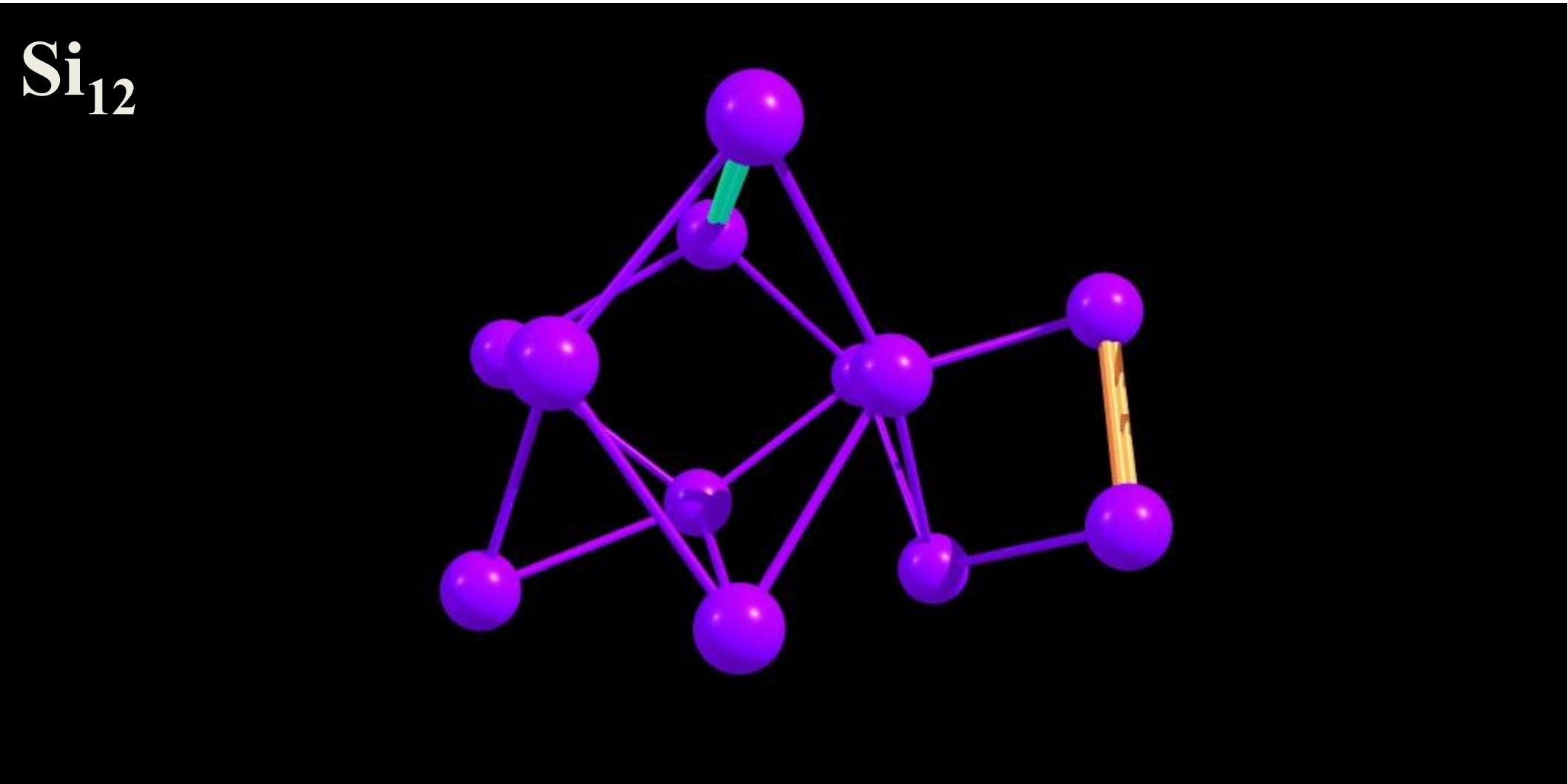


Marching tetrahedra

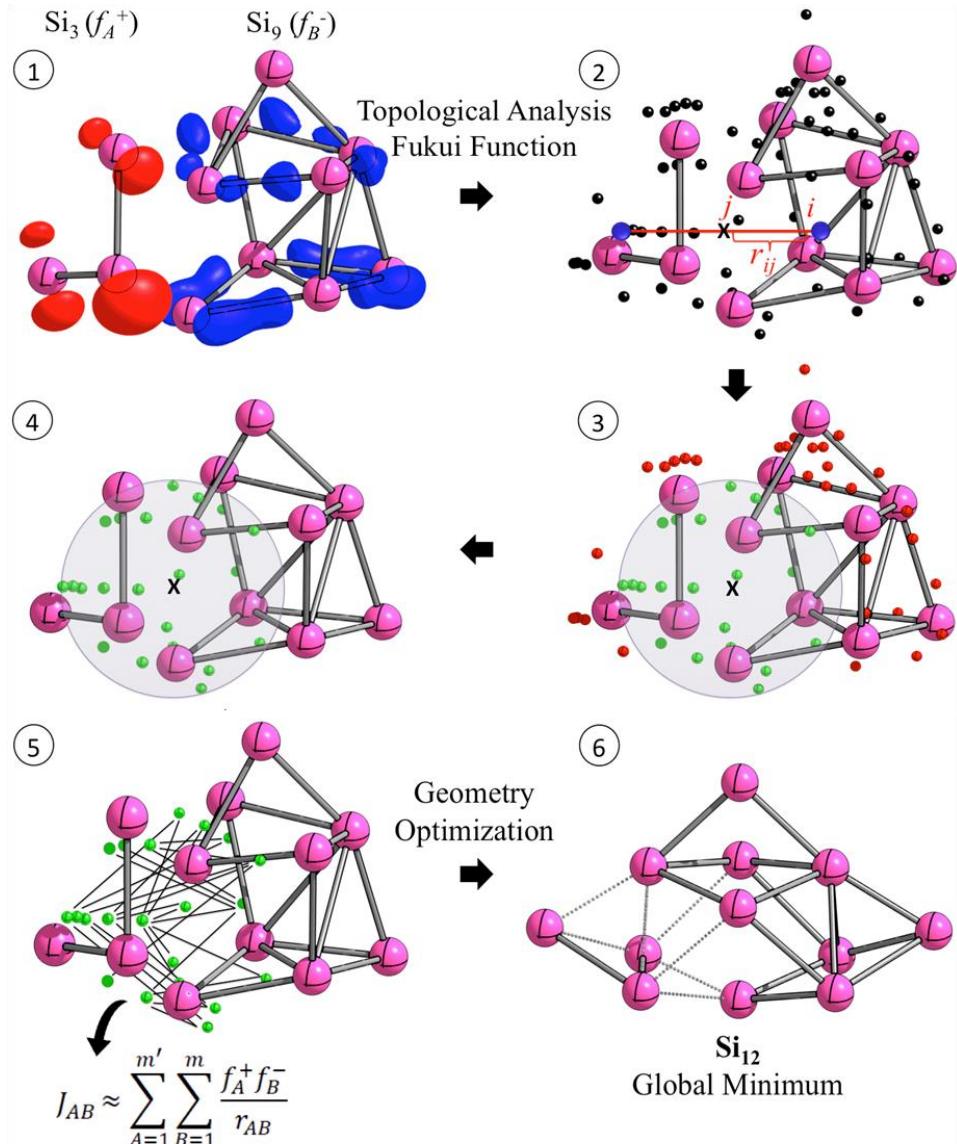


$$JV_{AB} = \sum_{i \in B} \sum_{j \in B} \frac{V_A^+(i)V_B^-(j)}{r_{ij}} + \sum_{k \in B} \sum_{l \in B} \frac{V_A^+(k)V_B^-(l)}{r_{kl}} + \sum_{i \in B} \sum_{l \in B} \frac{V_A^+(i)V_B^-(l)}{r_{il}} + \sum_{k \in B} \sum_{j \in B} \frac{V_A^+(k)V_B^-(j)}{r_{kj}}$$



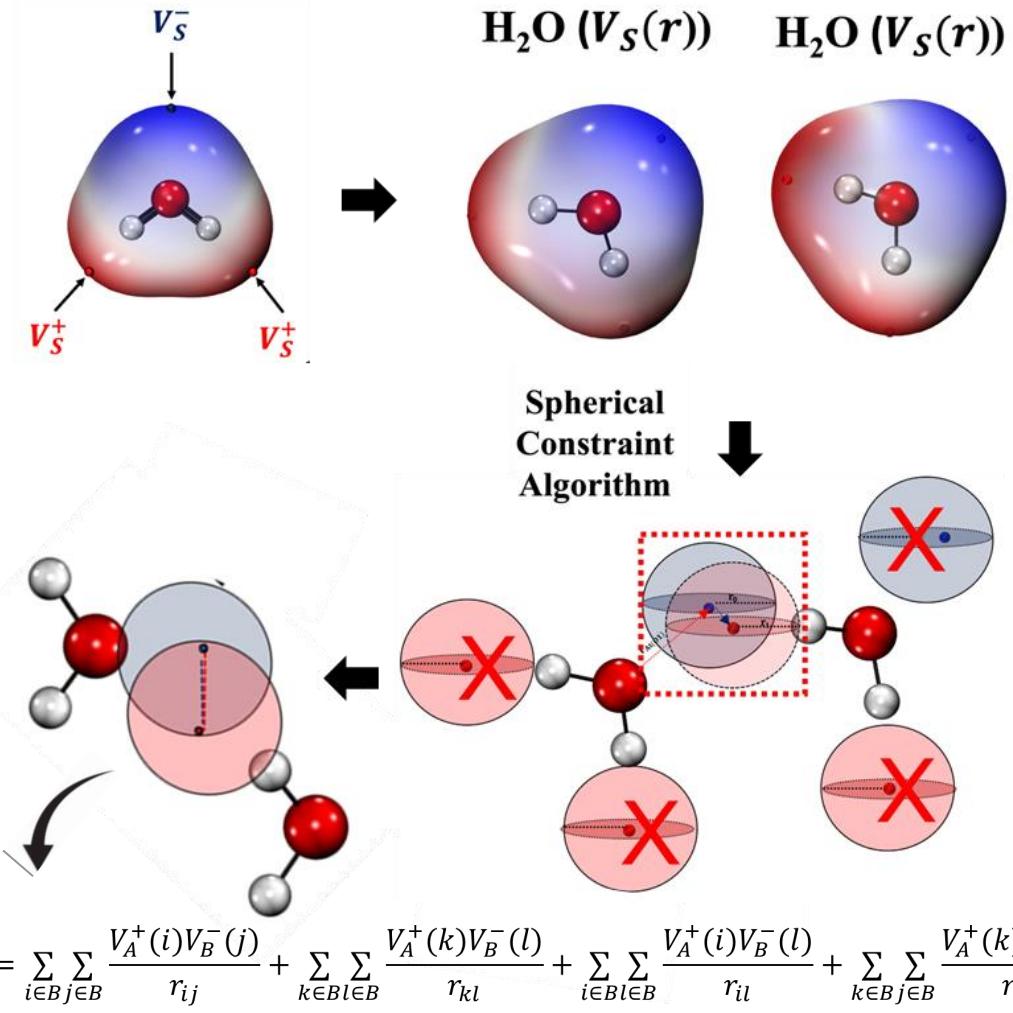


Constraint algorithms



Kick-Fukui

Calculation of the Molecular Electrostatic Surface Potencial



Kick-Mep



Kick–Fukui: A Fukui Function-Guided Method for Molecular Structure Prediction

Osvaldo Yañez, Rodrigo Báez-Grez, Diego Inostroza, Ricardo Pino-Rios, Walter A. Rabanal-León, Julia Contreras-García,* Carlos Cardenas,* and William Tiznado*

Cite This: *J. Chem. Inf. Model.* 2021, 61, 3955–3963

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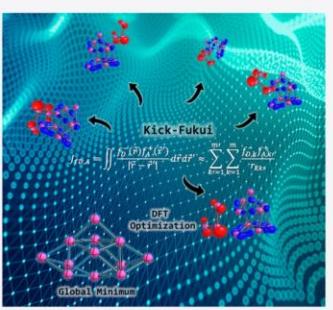
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ABSTRACT: Here, we introduce a hybrid method, named Kick–Fukui, to explore the potential energy surface (PES) of clusters and molecules using the Coulombic integral between the Fukui functions in the first screening of the best individuals. In the process, small stable molecules or clusters whose combination has the stoichiometry of the explored species are used as assembly units. First, a small set of candidates has been selected from a large and stochastically generated (Kick) population according to the maximum value of the Coulombic integral between the Fukui functions of both fragments. Subsequently, these few candidates are optimized using a gradient method and density functional theory (DFT) calculations. The performance of the program has been evaluated to explore the PES of various systems, including atomic and molecular clusters. In most cases studied, the global minimum (GM) has been identified with a low computational cost. The strategy does not allow to identify the GM of some silicon clusters; however, it predicts local minima very close in energy to the GM that could be used as the initial population of evolutionary algorithms.



Journal of Molecular Modeling (2024) 30:369
<https://doi.org/10.1007/s00894-024-06155-0>

ORIGINAL PAPER

Introducing KICK-MEP: exploring potential energy surfaces in systems with significant non-covalent interactions

Williams García-Argote^{1,2} · Lina Ruiz³ · Diego Inostroza¹ · Carlos Cardenas^{4,5} · Osvaldo Yañez⁶ · William Tiznado¹

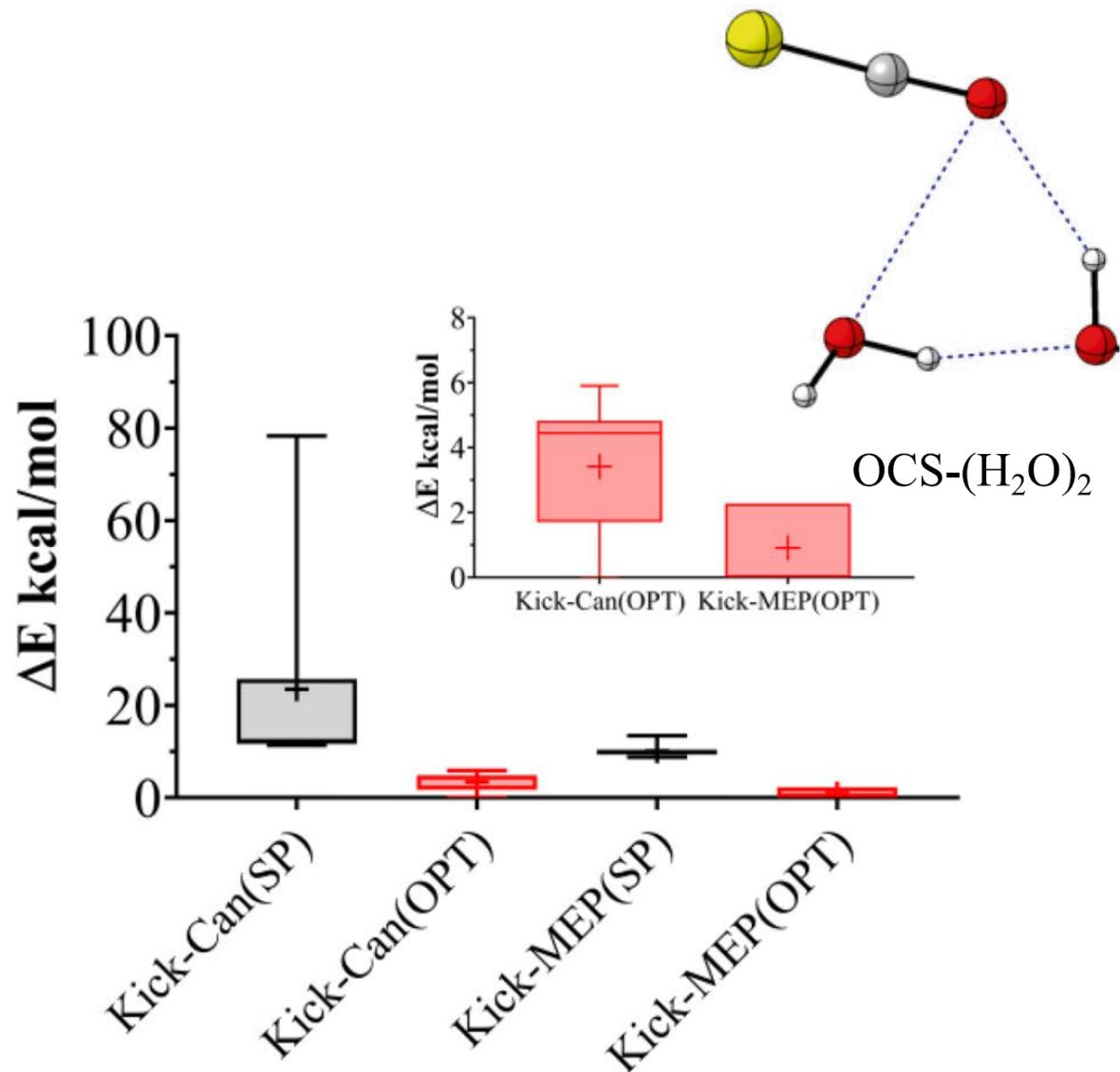
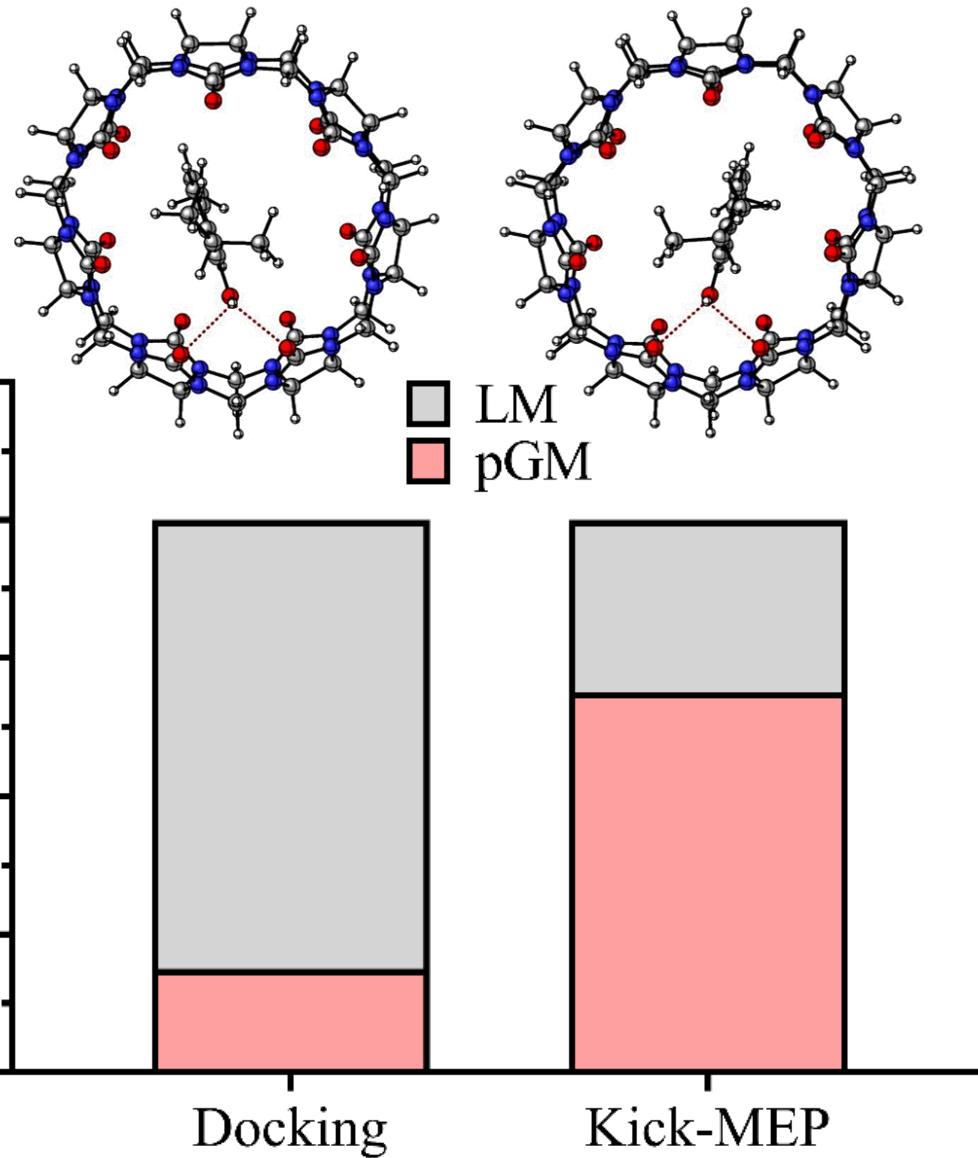
Received: 2 June 2024 / Accepted: 20 September 2024

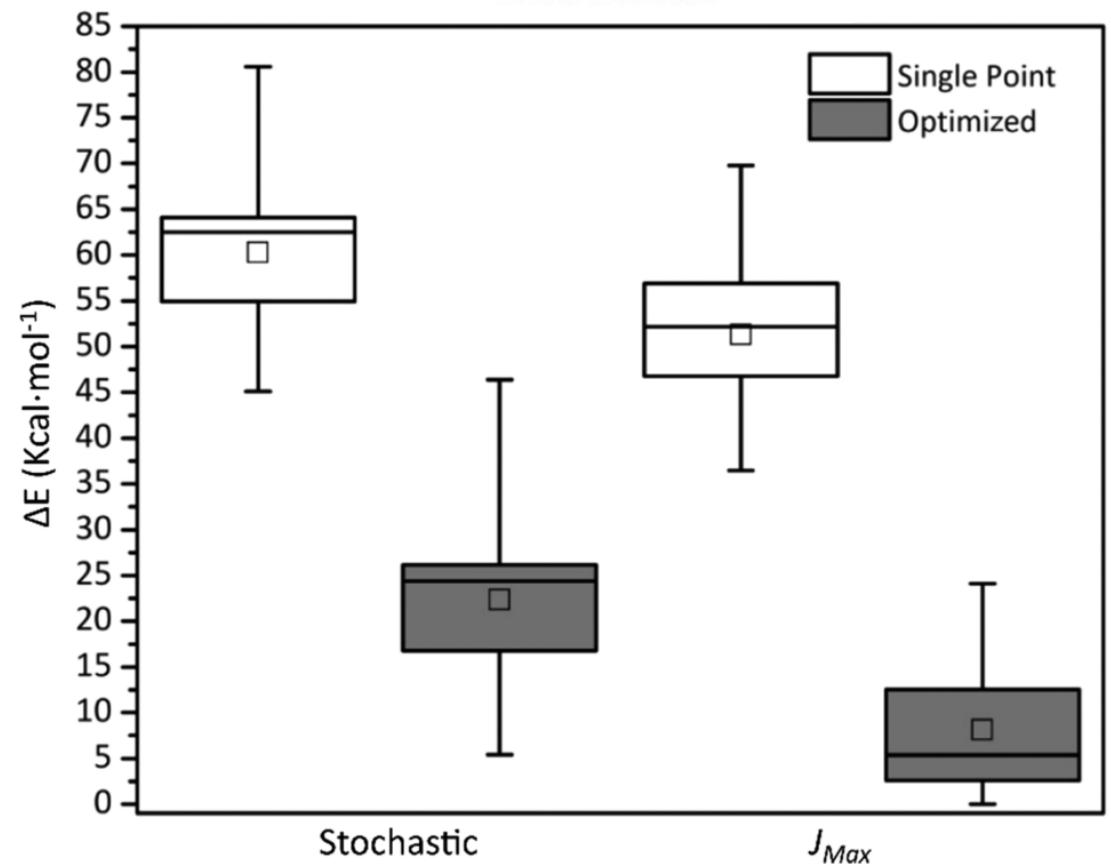
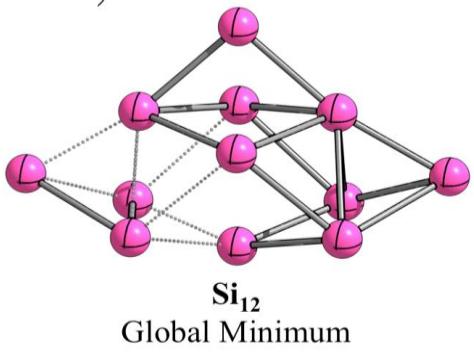
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Abstract

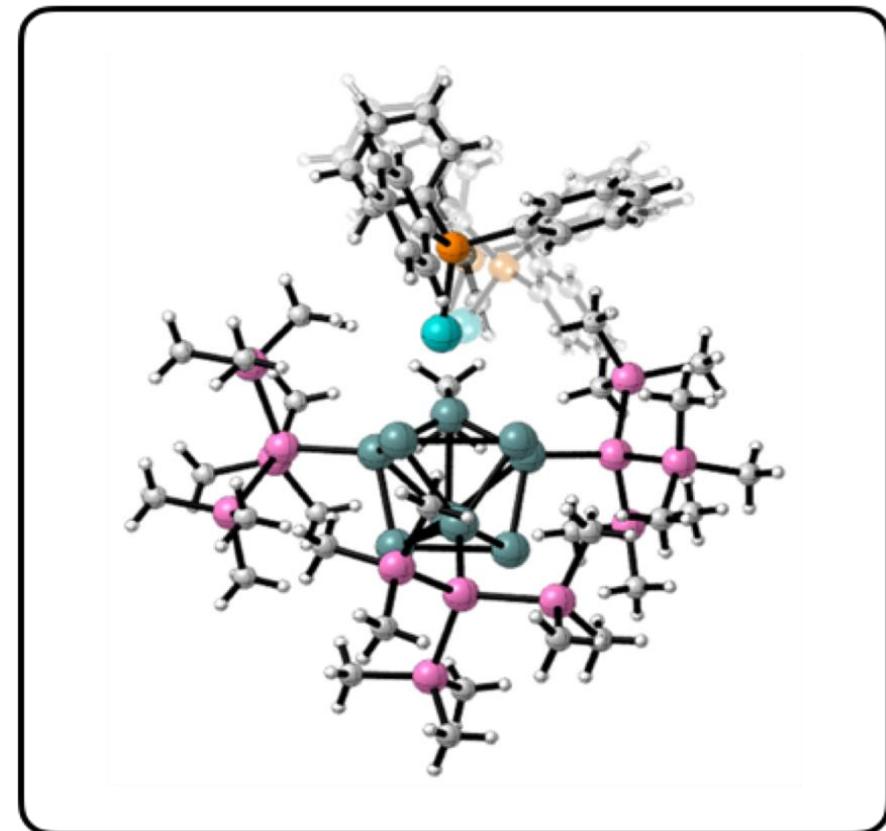
Context Exploring potential energy surfaces (PES) is fundamental in computational chemistry, as it provides insights into the relationship between molecular energy, geometry, and chemical reactivity. We introduce Kick-MEP, a hybrid method for exploring the PES of atomic and molecular clusters, particularly those dominated by non-covalent interactions. Kick-MEP computes the Coulomb integral between the maximum and minimum electrostatic potential values on a 0.001 a.u. electron density isosurface for two interacting fragments. This approach efficiently estimates interaction energies and selects low-energy configurations at reduced computational cost. Kick-MEP was evaluated on silicon-lithium clusters, water clusters, and thymol encapsulated within Cucurbit[7]uril, consistently identifying the lowest energy structures, including global minima and relevant local minima.

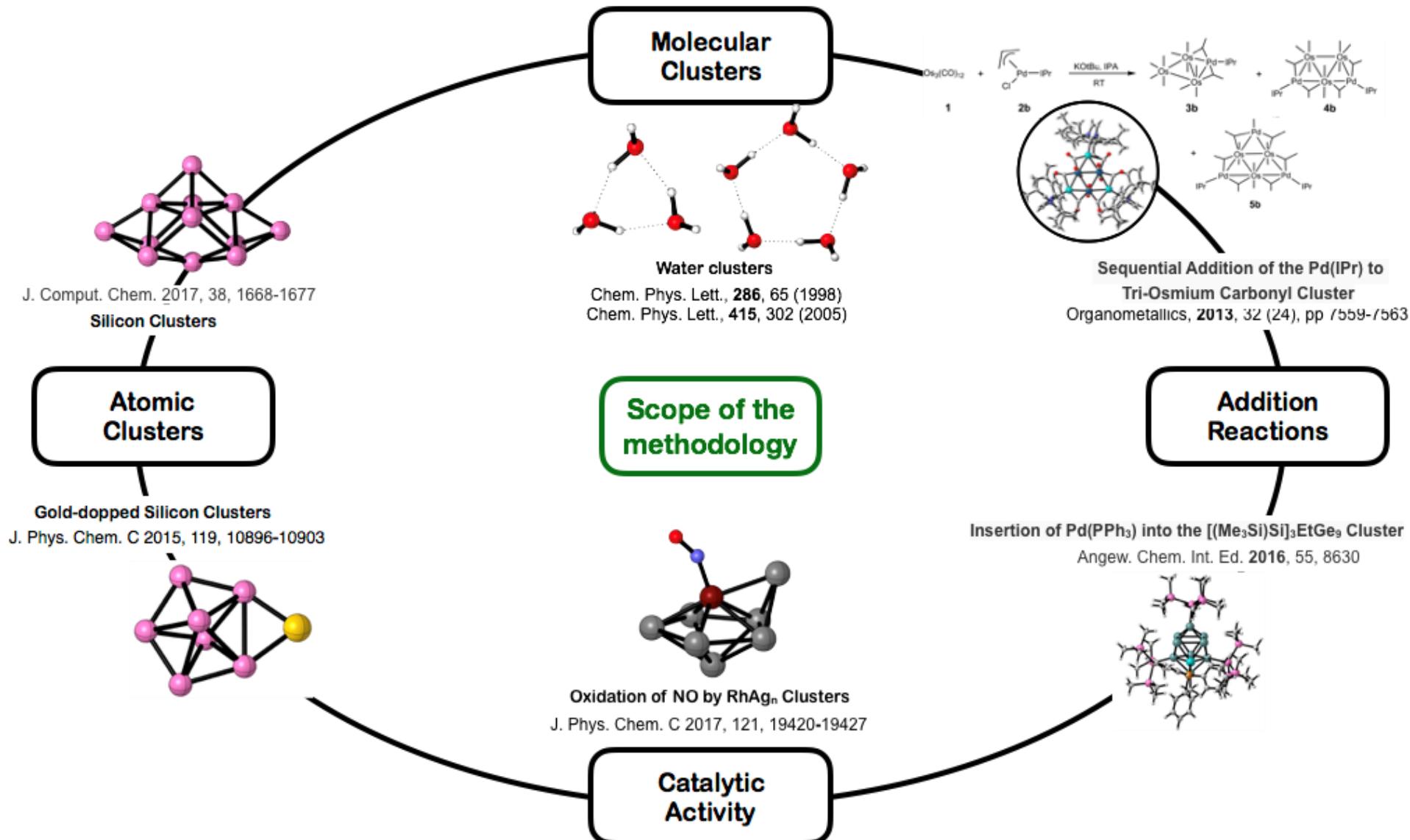
Thymol@Curcubit[7]uril





Insertion of $\text{Pd}(\text{PPh}_3)$ into the $[(\text{Me}_3\text{Si})\text{Si}]_3\text{-EtGe}_9$ cluster







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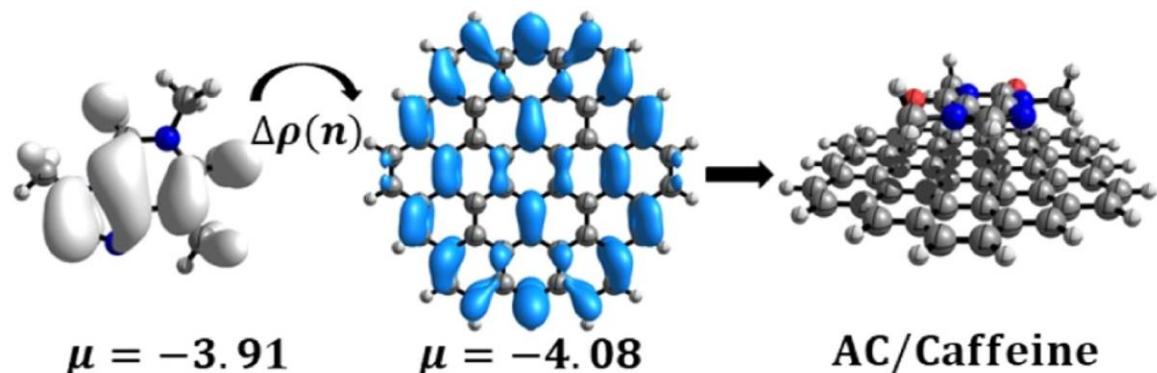
Journal of Environmental Chemical Engineering

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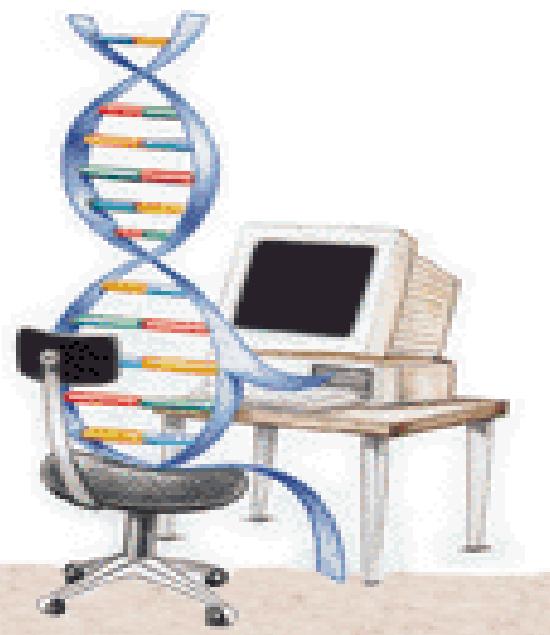
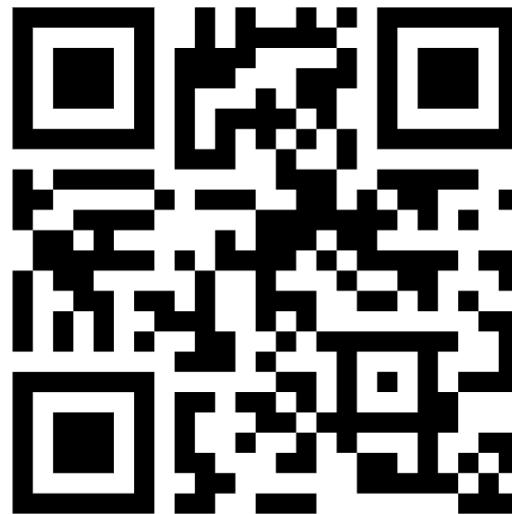
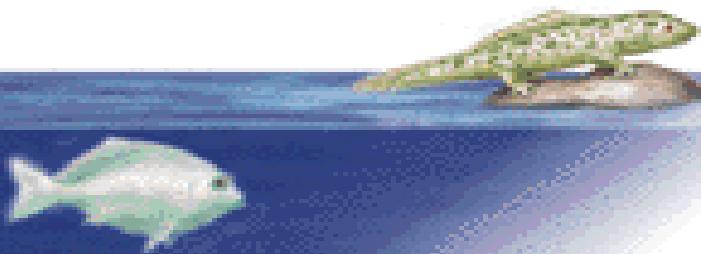


Exploring the adsorption of five emerging pollutants on activated carbon: A theoretical approach

Lisdelys González-Rodríguez ^{a,b}, Osvaldo Yáñez ^b, Karel Mena- Ulecia ^{c,d}, Yoan Hidalgo-Rosa ^{e,f}, Ximena García- Carmona ^g, Claudia Ulloa- Tesser ^{h,*}



My GitHub repository



Acknowledgement



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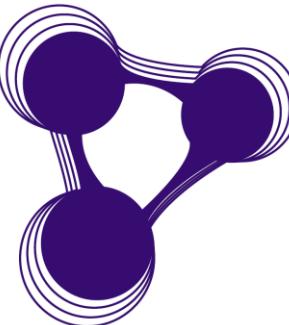
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