

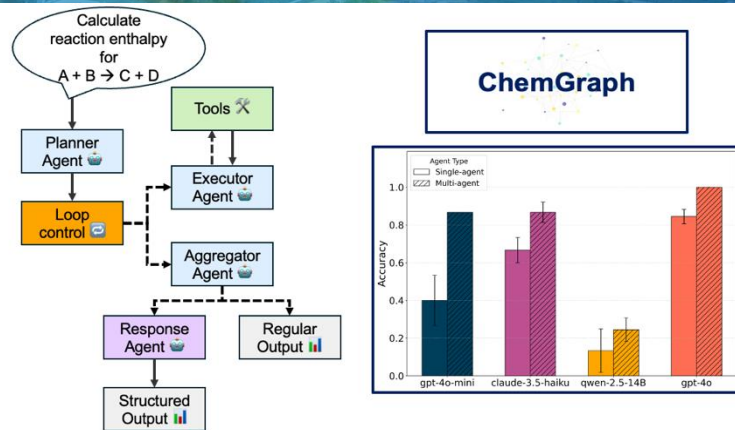
OCTOBER 28, 2025

CHEMGRAPH: AN AGENTIC AI FRAMEWORK FOR COMPUTATIONAL CHEMISTRY WORKFLOWS

THANG PHAM¹, ADITYA TANIKANTI², MURAT KEÇELI¹

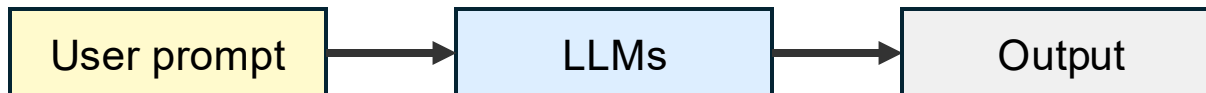
¹Computational Science (CPS) Division, Argonne National Laboratory

²Argonne Leadership Facility Computing, Argonne National Laboratory

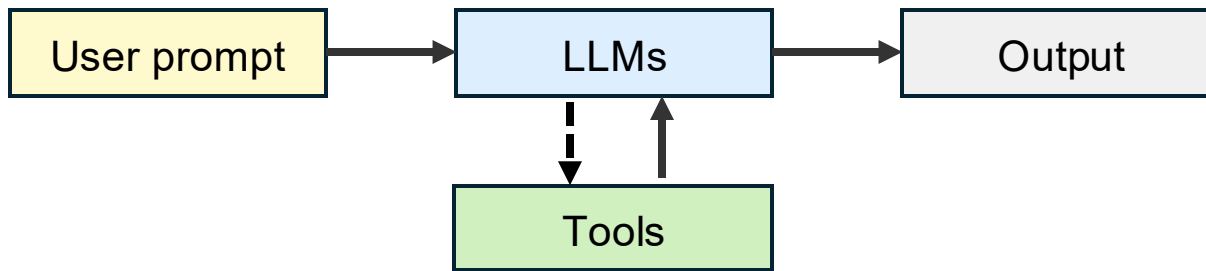


Large Language Models and Agentic AI

Large language models (LLMs):



Agentic AI:



Hallucinations in LLMs

Human

Provide the SMILES string corresponding to this molecule: 9-[(2,6-dichlorophenyl)methyl]-N-(furan-2-ylmethyl)purin-6-amine

LLMs (with GPT-4o)

The molecule **9-[(2,6-dichlorophenyl)methyl]-N-(furan-2-ylmethyl)purin-6-amine** has the following structure components:

- A **purine** core
- Substitution at position 9: a **(2,6-dichlorophenyl)methyl** group
- Substitution at position 6: an **amino group**
- That **amino group** is further substituted with a **furan-2-ylmethyl** group

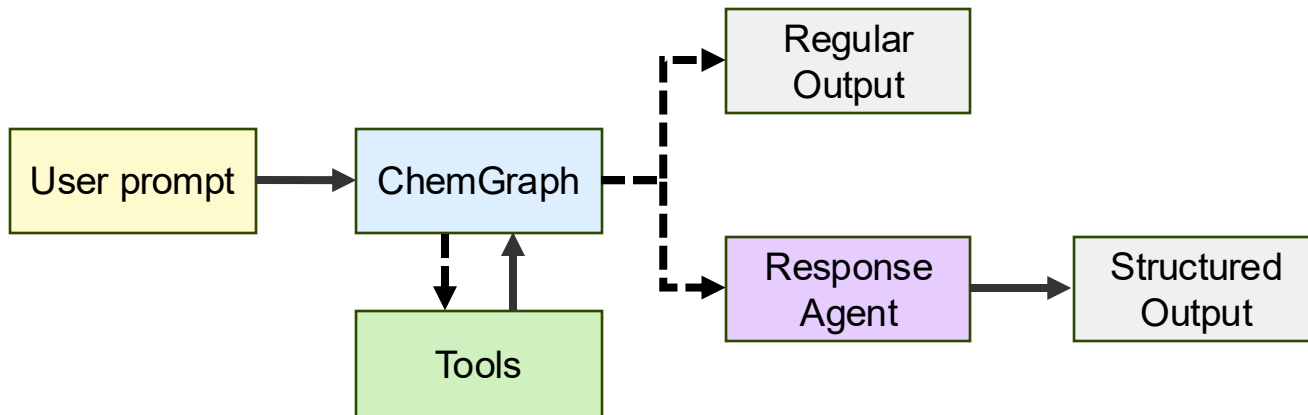
Constructed SMILES:

Incorrect

Clc1cccc(Cl)c1CN2c3nc(nc(NCC4=CC=CO4)c3nc2)N

[...]

ChemGraph: An Agentic Framework for Computational Chemistry



Software suite



Pham, T. D.; Tanikanti, A.; Keçeli, M. <https://arxiv.org/abs/2506.06363>

ChemGraph Solves Problems using Tools

Human

Provide the SMILES string corresponding to this molecule: 9-[(2,6-dichlorophenyl)methyl]-N-(furan-2-ylmethyl)purin-6-amine

LLMs (with GPT-4o)

The molecule **9-[(2,6-dichlorophenyl)methyl]-N-(furan-2-ylmethyl)purin-6-amine** has the following structure components:

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Constructed SMILES: Incorrect

Clc1cccc(Cl)c1CN2c3nc(nc(NCC4=CC=CO4)c3nc2)N

[...]

ChemGraph (with GPT-4o-mini)

Tool Call:

Tool name: molecule_name_to_smiles

Args: 9-[(2,6-dichlorophenyl)methyl]-N-(furan-2-ylmethyl)purin-6-amine

Output:

"C1=CC(=C(C(=C1)Cl)CN2C=NC3=C(N=CN=C32)NCC4=CC=CO4)Cl"

The SMILES string corresponding to the molecule "9-[(2,6-dichlorophenyl)methyl]-N-(furan-2-ylmethyl)purin-6-amine" is Correct

C1=CC(=C(C(=C1)Cl)CN2C=NC3=C(N=CN=C32)NCC4=CC=CO4)Cl

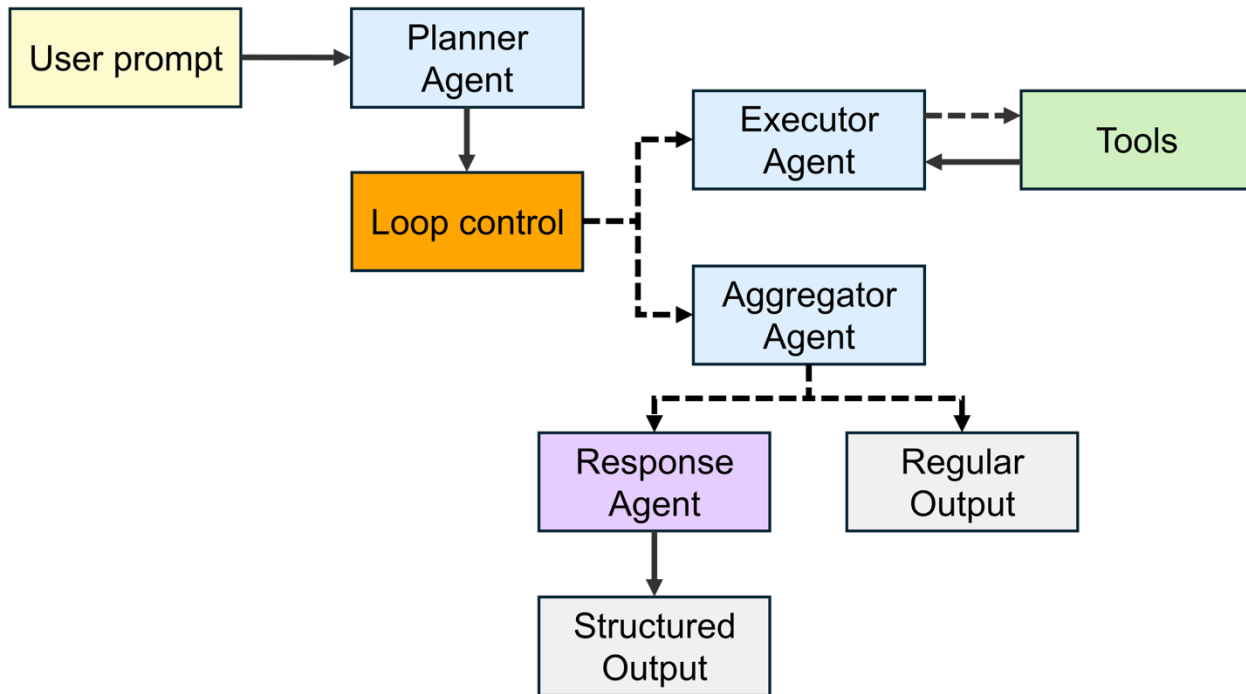
Evaluate ChemGraph Single-agent



** 360 tasks, more than 200 different molecules

Pham, T. D.; Tanikanti, A.; Keçeli, M. <https://arxiv.org/abs/2506.06363>

Multi-agent ChemGraph



Pham, T. D.; Tanikanti, A.; Keçeli, M. <https://arxiv.org/abs/2506.06363>



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Human and Multi-agent ChemGraph Interaction

Human

You are given a chemical reaction: 1 (Methane) + 2 (Oxygen) -> 1 (Carbon dioxide) + 2 (Water). Calculate the enthalpy change for this reaction using GFN2-xTB at 400K.

ChemGraph (multi-agent, GPT-4o-mini)

Planner agent

Task 1: Calculate the enthalpy of formation of methane (CH₄) using GFN2-xTB at 400K

Task 2: Calculate the enthalpy of formation of oxygen (O₂) using GFN2-xTB at 400K

Task 3: Calculate the enthalpy of formation of carbon dioxide (CO₂) using GFN2-xTB at 400K

Task 4: Calculate the enthalpy of formation of water (H₂O) using GFN2-xTB at 400K

Executor agents

Executor 1

Executor 2

Executor 3

Executor 4

Tool calls

Tool call 1: molecule_name_to_smiles(Methane)
Tool call 2: smiles_to_atmsdata("C")
Tool call 3: run_ase(Atomsdata(Methane),
driver=thermo, temperature=400,
"calculator"={"calculator_type": "TBLite",
"method": "GFN2-xTB"})

Tool outputs

The thermochemical calculation for methane (CH₄) using the GFN2-xTB method at 400K has been successfully completed [...]
Enthalpy of Formation: -112.2512 eV
[...]

[...]
Enthalpy of Formation: -214.93 eV
[...]

[...]
Enthalpy of Formation: -280.0425 eV
[...]

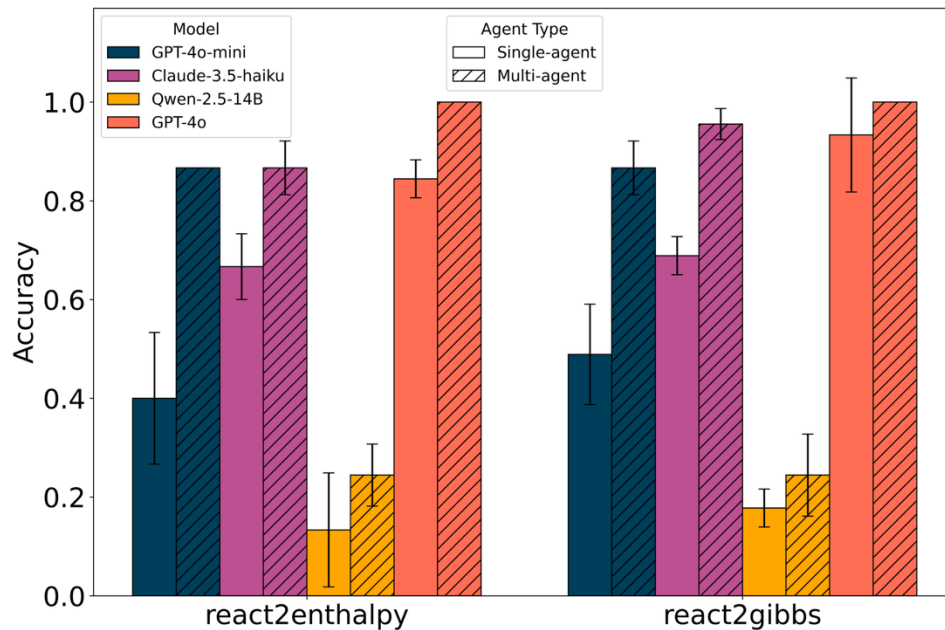
[...]
Enthalpy of Formation: -137.2903 eV
[...]

Aggregator agent

[...] Thus, the enthalpy change (u0394H) for the reaction is: Delta H = -12.5119 eV



Evaluate Chemgraph Multi-agent



Pham, T. D.; Tanikanti, A.; Keçeli, M. <https://arxiv.org/abs/2506.06363>



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ChemGraph User Interface

**ChemGraph**

Navigate

 Main Interface

 Configuration

 About ChemGraph

Quick Settings

Reload Config

 Agent Status

Agents Ready

Model: gemini-2.5-flash

Workflow: multi_agent

Thread ID: 1

Messages: 1

Refresh Agents

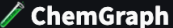
 Configuration

Use the Configuration page to modify settings, API endpoints, and chemistry parameters.

Current config loaded from: `config_tool`

Deploy

3D visualization is available via stmol.

**ChemGraph**

ChemGraph enables you to perform various computational chemistry tasks with natural-language queries using AI agents.

Conversation History

You:

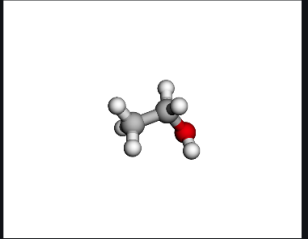
Calculate the IR spectrum of ethanol with a tight binding method

ChemGraph:

The IR spectrum of ethanol has been calculated using TBLite.
The calculated vibrational frequencies are (in cm^{-1}):
22.98, 10.97, 1.77, 0.07, 1.20, 9.07, 224.21, 340.44, 420.26, 831.00, 931.93, 1045.03, 1090.06, 1130.11, 1235.22, 1314.05, 1349.50, 1404.92, 1482.97, 1489.81, 1497.03, 2868.59, 2983.30, 3018.04, 3044.91, 3048.50, 3543.19.
An IR plot has been saved to "ir_spectrum.png" and normal mode data has been saved as individual ".traj" files.

Molecular Structure (Query 1)

Visualization Style
ball_and_stick



Structure Information

Atoms: 9

Formula: C2H6O

Composition:

+ C: 2

+ H: 6

+ O: 1

Total Mass: 46.07 amu

Center of Mass:
[0.318, -0.070, -0.234] Å

Additional Properties

Download:

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ChemGraph Capabilities: Current & Emerging

- Simulation engines
 - Density functional theory (DFT).
 - Foundation models (MACE, UMA).
 - Grand canonical Monte Carlo (GCMC).
- Agentic & Multimodal Intelligence
 - Constructions of metal-organic frameworks (MOFs) and organometallic compounds.
- HPC & Workflow Orchestration
 - Job submission.
 - Parsl.
- Open source: <https://github.com/argonne-lcf/ChemGraph>



THANK YOU FOR YOUR ATTENTION!



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