Towards Fully Automated Molecular Simulations: Multi-Agent Framework for Simulation Setup and Force Field Extraction

Marko Petković
Applied Physics and Science Education
Eindhoven University of Technology

Vlado Menkovski
Mathematics and Computer Science
Eindhoven University of Technology

Sofía Calero
Applied Physics and Science Education
Eindhoven University of Technology
{m.petkovic1, v.menkovski, s.calero}@tue.nl

Abstract

Automated characterization of porous materials has the potential to accelerate materials discovery, but it remains limited by the complexity of simulation setup and force field selection. We propose a multi-agent framework in which LLM-based agents can autonomously understand a characterization task, plan appropriate simulations, assemble relevant force fields, execute them and interpret their results to guide subsequent steps. As a first step toward this vision, we present a multi-agent system for literature-informed force field extraction and automated RASPA simulation setup. Initial evaluations demonstrate high correctness and reproducibility, highlighting this approach's potential to enable fully autonomous, scalable materials characterization.

1 Introduction

Porous materials, such as metal–organic frameworks (MOFs) and zeolites, are central to applications in energy storage, gas separation, catalysis, and carbon capture [9, 17, 21]. The design of novel porous materials with improved performance can have significant societal and environmental benefits. Molecular simulations play an important role in this process, as they provide molecular-level insights into adsorption and diffusion that are often inaccessible to experiments [10, 13, 30]. By revealing how structural features influence adsorption and transport, simulations can identify promising candidates and guide experimental efforts, thereby accelerating the discovery of porous materials [8, 36].

The adoption of molecular simulations for porous materials is limited by several technical challenges. Outcomes are highly sensitive to the choice of force fields and charge assignment methods, with studies showing that different protocols can result in markedly different adsorption predictions and even alter material rankings [7]. Maintaining reproducibility is also difficult, as variations in workflows, such as charge schemes, cutoff definitions, or structure curation, may hinder cross-study comparability [25]. Moreover, the diversity of force fields and their associated parameters requires deep expertise to select and apply them correctly [15]. These challenges create a barrier for wider use of simulations as a routine characterization tool.

Automated characterization of porous materials presents a multifaceted challenge, primarily due to the necessity for intelligent planning. Agents must determine the appropriate simulations to conduct, adapt workflows based on interim results, select or design accurate force fields, and generalize across diverse topologies, adsorbates, and conditions. Recent advances in large language models

Preprint.

(LLMs) have demonstrated their capability to address these complexities [3, 23, 26, 29]. LLMs have been shown to effectively generate structured workflows, interpret complex scientific tasks and synthesize executable simulation code, thereby facilitating the automation of intricate scientific processes [11, 37, 39, 41]. Their proficiency in integrating heterogeneous knowledge and performing flexible reasoning and multi-step planning makes them well-suited for orchestrating the adaptive workflows required in materials characterization [4, 20]. Furthermore, LLMs have been utilized to automate research workflows, including experimental protocol planning and scientific code generation, underscoring their potential in scientific automation [6, 22, 27, 35].

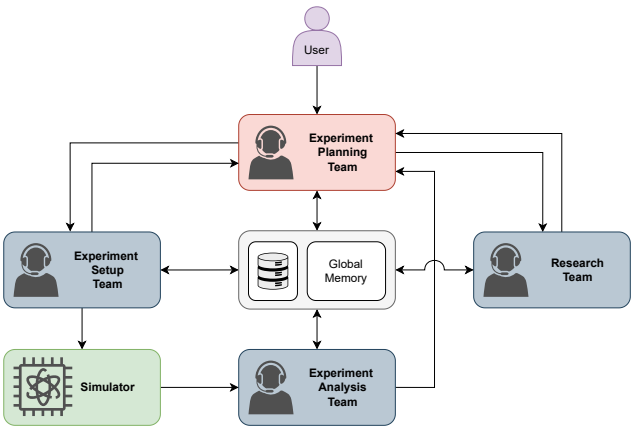

Figure 1: Vision of an autonomous multi-agent system for molecular simulations. The Experiment Planning Team coordinates research, setup, and analysis teams through a shared global memory, enabling iterative workflows in which user queries result in literature-derived force fields, RASPA simulations, and analysis of results.

Our goal is to develop a system that, given an experimental measurement or user request, can autonomously plan and execute the necessary steps to identify or design suitable force fields and then perform characterization simulations (Figure 1). By automating both the selection of physically accurate force fields and the execution of complex simulation workflows, such a system bridges experimental observations with predictive, simulation-driven insights. This approach not only reduces the expertise and time required to perform high-quality simulations but also enables routine, reproducible characterization of porous materials, accelerating materials discovery and guiding experiments with a level of efficiency and reliability that would be difficult to achieve manually.

As a step toward this vision, we present two key agent-based components that form the foundation of the system. First, experiment setup agents that can automatically generate RASPA [12] input files for increasingly complex characterization tasks, including adsorption isotherms, heats of adsorption, and multi-adsorbate or multi-structure scenarios. Second, force field retrieval agents that autonomously extract relevant parameters from the literature and convert them into a format ready for RASPA simulations. We evaluate the correctness and reliability of these components and discuss how they provide a scalable framework for fully automated characterization workflows in porous materials.

2 Methods

Our system is organized into two specialized teams of LLM-based agents, using the ReAct framework [38], that collaboratively perform autonomous materials characterization. The experiment setup team (Figure 2) is coordinated by a supervisor agent that processes user or experimental requests and sets up the corresponding simulations. The supervisor delegates responsibilities to specialized agents: a structure agent identifies and prepares relevant structure copies, a force field agent combines and formats appropriate force field files, a simulation input agent generates templated RASPA input files, and a code generation agent [34] automates file operations and template creation. After each agent completes its task, an evaluator agent [40] inspects the generated outputs and provides feedback to ensure correctness and consistency. Agents have access to general tools for file manipulation, while relevant agents also use functions to extract information from files without opening them directly.

In addition, they share a global memory, which each agent can update with structured reports of task execution and outputs. Furthermore, agents have access to example input files from the RASPA manual, as well as a library containing multiple force fields to base their simulations on.

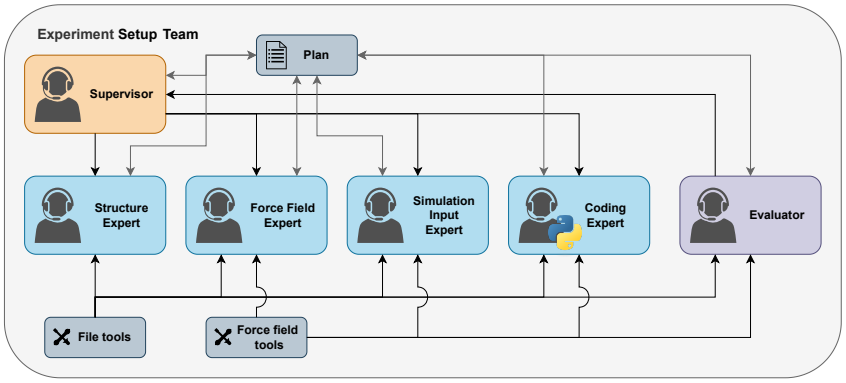

Figure 2: Experiment Setup Team overview.

The paper research team (Figure 3) extracts simulation-relevant knowledge from the literature. A paper search agent retrieves relevant publications, which are passed to an extraction agent that reads the papers and summarizes key findings related to force field parameters. A force field writer agent then converts these findings into simulation-ready force field files, and has access to dummy force field files to base the force fields on. Agents communicate iteratively, requesting additional information when needed (e.g., if a force field extends results from a different publication), ensuring accuracy and completeness of the extracted knowledge.

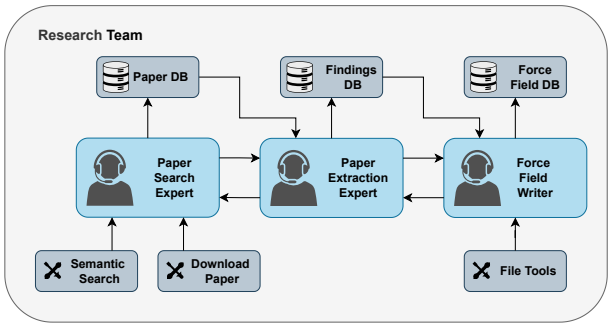

Figure 3: Research Team overview.

The agentic framework is implemented using LangChain and LangGraph. The paper search agent uses Semantic Scholar [1] for queries. The code for the experiments can be found in this repository, while more details on the agentic system can be found in Appendix A.

3 Experiments

To evaluate our simulation setup system, we designed a series of zeolite adsorption tasks with increasing complexity. These include adsorption isotherms and heats of adsorption (HOA) for single (CH_4) and multiple adsorbates (CH_4, CO_2, CO), as well as simulations spanning single and multiple zeolite structures. Each task is deliberately constructed so that agents must integrate input parameters from multiple sources, combining adsorbate properties and force field parameters from separate files, requiring correct assembly and templating. The system has access to several commonly used force fields for molecules in zeolites [5, 18, 24, 28], which agents retrieve or combine as needed. Each simulation setup is performed five times, and the resulting files are evaluated both manually and by executing them in RASPA to verify correctness and reproducibility.

To evaluate the paper research team, we select a set of publications and process each five times to assess reproducibility. The agents extract force field parameters from the papers, and we verify whether all relevant parameters are correctly identified and formatted for use in simulations.

Table 1: Experiment Setup Team results. For each task, the number of zeolite structures and adsorbates, as well as the success and execution rates, are shown.

Task	Str.	Ads.	Succ.	Exec.
Isotherm	1	1	100%	100%
		3	100%	100%
HOA	500	1	80%	100%
		3	80%	80%
Isotherm	500	1	100%	100%
		3	80%	100%

Table 2: Research Team results. For each force field, the average number of missed parameters, wrong parameters, and the Intersection over Union (IoU) between extracted and correct parameters are shown.

Force fields	Missed	Wrong	IoU
CO_2 [18]	0	0	1.00
TraPPE-zeo [2]	0	0.6	0.90
CO_2 N_2 O_2 Ar [33]	0	1.4	0.96
EPM2 (CO_2) [19]	0	3	0.67
CO_2 [14]	0	1	0.96
C_xH_x CO_2 N_2 O_2 [16]	0	0	1.00

Overall, the system performed well in the experiment setup task (Table 1), with a high rate of successful and executable simulations. We define the success rate as the proportion of simulations correctly configured for their intended task, and the execution rate as the proportion that run without errors. The few failures we observed came from specific issues: in the isotherm case with three adsorbates, the setup incorrectly generated a combined mixture simulation instead of three individual simulations; the Widom insertion method was not configured correctly for single-adsorbate HOA; and for three adsorbates, the framework file was not copied. We also observed certain decisions, such as selecting a non-standard cutoff (24 Å instead of the typical 12 Å) or enforcing minimum unit cells in each direction, that were unusual but still led to correct and runnable simulations. Additional details on the simulation setups, including deviations and encountered issues, are provided in Appendix B.

Table 2 shows the performance of the Research Team in extracting force field parameters. Across all tested cases, no parameters were entirely missed, indicating high recall. Most errors arose from incorrect numerical values being assigned to otherwise correct terms. In the case of TraPPE-zeo, the model introduced a non-existent interaction term. For EPM2, all numbers were extracted correctly but assigned to the wrong interactions due to the unconventional table layout, which reduced the Intersection over Union (IoU) to 0.67. For the other force fields, the IoU remained high (≥ 0.9), showing that the system is generally reliable when parameter tables follow standard formats.

In addition to the independent experiments, we conducted a coordinated experiment in which the two teams were overseen by a supervisor. They were tasked with extracting the force field from [18] and setting up an adsorption isotherm simulation for a structure using the extracted force field. The system successfully completed this workflow. An overview of the execution is in Appendix C.

4 Discussion

Our results demonstrate that autonomous agents can reliably set up molecular simulations and extract force field parameters from the literature, with only a small number of task-specific errors. These outcomes suggest that multi-agent systems provide a promising foundation for automated characterization of porous materials.

Looking forward, the most significant opportunity lies in equipping agent-based systems with structured, persistent memory representations. At present, knowledge is encoded procedurally in prompts and tools, limiting the ability of agents to adapt across tasks or to refine strategies based on past experience. Incorporating semantic memory (e.g., domain-specific heuristics that experts apply when setting up simulations) and episodic memory could enable more consistent and generalizable behavior [20, 31, 40]. This would allow agents to construct increasingly sophisticated workflows for materials characterization, bridging experimental observations with predictive modeling in a continuous loop. Ultimately, such systems could serve as the foundation for self-driving laboratories [32], where simulation and experimentation workflows are autonomously integrated in real time to accelerate the discovery of high-performance porous materials.

References

[1] Waleed Ammar, Dirk Groeneveld, Chandra Bhagavatula, Iz Beltagy, Miles Crawford, Doug Downey, Jason Dunkelberger, Ahmed Elgohary, Sergey Feldman, Vu Ha, et al. Construction of the literature graph in semantic scholar. *arXiv preprint arXiv:1805.02262*, 2018.

[2] Peng Bai, Michael Tsapatsis, and J Ilja Siepmann. Trappe-zeo: Transferable potentials for phase equilibria force field for all-silica zeolites. *The Journal of Physical Chemistry C*, 117(46):24375–24387, 2013.

[3] Daniil A Boiko, Robert MacKnight, Ben Kline, and Gabe Gomes. Autonomous chemical research with large language models. *Nature*, 624(7992):570–578, 2023.

[4] Sébastien Bubeck, Varun Chandrasekaran, Ronen Eldan, Johannes Gehrke, Eric Horvitz, Ece Kamar, Peter Lee, Yin Tat Lee, Yuanzhi Li, Scott Lundberg, et al. Sparks of artificial general intelligence: Early experiments with gpt-4. *arXiv preprint arXiv:2303.12712*, 2023.

[5] Sofía Calero, David Dubbeldam, Rajamani Krishna, Berend Smit, Thijs JH Vlugt, Joeri FM Denayer, Johan A Martens, and Theo LM Maesen. Understanding the role of sodium during adsorption: a force field for alkanes in sodium-exchanged faujasites. *Journal of the American Chemical Society*, 126(36):11377–11386, 2004.

[6] Pengfei Cao, Tianyi Men, Wencan Liu, Jingwen Zhang, Xuzhao Li, Xixun Lin, Dianbo Sui, Yanan Cao, Kang Liu, and Jun Zhao. Large language models for planning: A comprehensive and systematic survey. *arXiv preprint arXiv:2505.19683*, 2025.

[7] Conor Cleeton, Felipe Lopes De Oliveira, Rodrigo F Neumann, Amir H Farmahini, Binquan Luan, Mathias Steiner, and Lev Sarkisov. A process-level perspective of the impact of molecular force fields on the computational screening of mofs for carbon capture. *Energy & Environmental Science*, 16(9):3899–3918, 2023.

[8] Yamil J Colón and Randall Q Snurr. High-throughput computational screening of metal–organic frameworks. *Chemical Society Reviews*, 43(16):5735–5749, 2014.

[9] Avelino Corma. From microporous to mesoporous molecular sieve materials and their use in catalysis. *Chemical reviews*, 97(6):2373–2420, 1997.

[10] François-Xavier Coudert. Responsive metal–organic frameworks and framework materials: under pressure, taking the heat, in the spotlight, with friends. *Chemistry of Materials*, 27(6):1905–1916, 2015.

[11] Kourosh Darvish, Marta Skreta, Yuchi Zhao, Naruki Yoshikawa, Sagnik Som, Miroslav Bogdanovic, Yang Cao, Han Hao, Haoping Xu, Alán Aspuru-Guzik, et al. Organa: A robotic assistant for automated chemistry experimentation and characterization. *Matter*, 8(2), 2025.

[12] David Dubbeldam, Sofía Calero, Donald E Ellis, and Randall Q Snurr. Raspa: molecular simulation software for adsorption and diffusion in flexible nanoporous materials. *Molecular Simulation*, 42(2):81–101, 2016.

[13] Tina Düren, Franck Millange, Gérard Férey, Krista S Walton, and Randall Q Snurr. Calculating geometric surface areas as a characterization tool for metal- organic frameworks. *The Journal of Physical Chemistry C*, 111(42):15350–15356, 2007.

[14] Hanjun Fang, Preeti Kamakoti, Peter I Ravikovitch, Matthew Aronson, Charanjit Paur, and David S Sholl. First principles derived, transferable force fields for co 2 adsorption in na-exchanged cationic zeolites. *Physical Chemistry Chemical Physics*, 15(31):12882–12894, 2013.

[15] Amir H Farmahini, Shreenath Krishnamurthy, Daniel Friedrich, Stefano Brandani, and Lev Sarkisov. Performance-based screening of porous materials for carbon capture. *Chemical Reviews*, 121(17):10666–10741, 2021.

[16] John M Findley, Salah Eddine Boulfelfel, Hanjun Fang, Giovanni Muraro, Peter I Ravikovitch, and David S Sholl. A transferable force field for predicting adsorption and diffusion of hydrocarbons and small molecules in silica zeolites with coupled-cluster accuracy. *The Journal of Physical Chemistry C*, 125(15):8418–8429, 2021.

[17] Hiroyasu Furukawa, Kyle E Cordova, Michael O'Keeffe, and Omar M Yaghi. The chemistry and applications of metal-organic frameworks. *Science*, 341(6149):1230444, 2013.

[18] Almudena Garcia-Sanchez, Conchi O Ania, José B Parra, David Dubbeldam, Thijs JH Vlugt, Rajamani Krishna, and Sofia Calero. Transferable force field for carbon dioxide adsorption in zeolites. *The Journal of Physical Chemistry C*, 113(20):8814–8820, 2009.

[19] Jonathan G Harris and Kwong H Yung. Carbon dioxide's liquid-vapor coexistence curve and critical properties as predicted by a simple molecular model. *The Journal of Physical Chemistry*, 99(31):12021–12024, 1995.

[20] Xu Huang, Weiwen Liu, Xiaolong Chen, Xingmei Wang, Hao Wang, Defu Lian, Yasheng Wang, Ruiming Tang, and Enhong Chen. Understanding the planning of llm agents: A survey. *arXiv preprint arXiv:2402.02716*, 2024.

[21] Jian-Rong Li, Ryan J Kuppler, and Hong-Cai Zhou. Selective gas adsorption and separation in metal–organic frameworks. *Chemical Society Reviews*, 38(5):1477–1504, 2009.

[22] Ziming Luo, Zonglin Yang, Zexin Xu, Wei Yang, and Xinya Du. Llm4sr: A survey on large language models for scientific research. *arXiv preprint arXiv:2501.04306*, 2025.

[23] Andres M. Bran, Sam Cox, Oliver Schilter, Carlo Baldassari, Andrew D White, and Philippe Schwaller. Augmenting large language models with chemistry tools. *Nature Machine Intelligence*, 6(5):525–535, 2024.

[24] Ana Martin-Calvo, JJ Gutiérrez-Sevillano, JB Parra, CO Ania, and Sofia Calero. Transferable force fields for adsorption of small gases in zeolites. *Physical Chemistry Chemical Physics*, 17(37):24048–24055, 2015.

[25] Daniele Ongari, Leopold Talirz, and Berend Smit. Too many materials and too many applications: an experimental problem waiting for a computational solution. *ACS central science*, 6(11):1890–1900, 2020.

[26] Mayk Caldas Ramos, Christopher J Collison, and Andrew D White. A review of large language models and autonomous agents in chemistry. *Chemical science*, 2025.

[27] Shuo Ren, Pu Jian, Zhenjiang Ren, Chunlin Leng, Can Xie, and Jiajun Zhang. Towards scientific intelligence: A survey of llm-based scientific agents. *arXiv preprint arXiv:2503.24047*, 2025.

[28] Pablo Romero-Marimon, Juan Jose Gutierrez-Sevillano, and Sofia Calero. Adsorption of carbon dioxide in non-löwenstein zeolites. *Chemistry of Materials*, 35(13):5222–5231, 2023.

[29] Yixiang Ruan, Chenyin Lu, Ning Xu, Yuchen He, Yixin Chen, Jian Zhang, Jun Xuan, Jianzhang Pan, Qun Fang, Hanyu Gao, et al. An automatic end-to-end chemical synthesis development platform powered by large language models. *Nature communications*, 15(1):10160, 2024.

[30] Berend Smit and Theo LM Maesen. Molecular simulations of zeolites: adsorption, diffusion, and shape selectivity. *Chemical reviews*, 108(10):4125–4184, 2008.

[31] Theodore Sumers, Shunyu Yao, Karthik Narasimhan, and Thomas Griffiths. Cognitive architectures for language agents. *Transactions on Machine Learning Research*, 2023.

[32] Gary Tom, Stefan P Schmid, Sterling G Baird, Yang Cao, Kourosh Darvish, Han Hao, Stanley Lo, Sergio Pablo-García, Ella M Rajaonson, Marta Skreta, et al. Self-driving laboratories for chemistry and materials science. *Chemical Reviews*, 124(16):9633–9732, 2024.

[33] Bojan Vujić and Alexander P Lyubartsev. Transferable force-field for modelling of co2, n2, o2 and ar in all silica and na+ exchanged zeolites. *Modelling and simulation in Materials science and Engineering*, 24(4):045002, 2016.

[34] Xingyao Wang, Yangyi Chen, Lifan Yuan, Yizhe Zhang, Yunzhu Li, Hao Peng, and Heng Ji. Executable code actions elicit better llm agents. In *Forty-first International Conference on Machine Learning*, 2024.

[35] Hui Wei, Zihao Zhang, Shenghua He, Tian Xia, Shijia Pan, and Fei Liu. Plangenllms: A modern survey of llm planning capabilities. *arXiv preprint arXiv:2502.11221*, 2025.

[36] Christopher E Wilmer, Michael Leaf, Chang Yeon Lee, Omar K Farha, Brad G Hauser, Joseph T Hupp, and Randall Q Snurr. Large-scale screening of hypothetical metal–organic frameworks. *Nature chemistry*, 4(2):83–89, 2012.

[37] Jia Xu, Weilin Du, Xiao Liu, and Xuejun Li. Llm4workflow: An llm-based automated workflow model generation tool. In *Proceedings of the 39th IEEE/ACM International Conference on Automated Software Engineering*, pages 2394–2398, 2024.

[38] Shunyu Yao, Jeffrey Zhao, Dian Yu, Nan Du, Izhak Shafran, Karthik Narasimhan, and Yuan Cao. React: Synergizing reasoning and acting in language models. In *International Conference on Learning Representations (ICLR)*, 2023.

[39] Naruki Yoshikawa, Marta Skreta, Kourosh Darvish, Sebastian Arellano-Rubach, Zhi Ji, Lasse Bjørn Kristensen, Andrew Zou Li, Yuchi Zhao, Haoping Xu, Artur Kuramshin, et al. Large language models for chemistry robotics. *Autonomous Robots*, 47(8):1057–1086, 2023.

[40] Mingchen Zhuge, Changsheng Zhao, Dylan Ashley, Wenyi Wang, Dmitrii Khizbullin, Yunyang Xiong, Zechun Liu, Ernie Chang, Raghuraman Krishnamoorthi, Yuandong Tian, et al. Agent-as-a-judge: Evaluate agents with agents. *arXiv preprint arXiv:2410.10934*, 2024.

[41] Yunheng Zou, Austin H Cheng, Abdulrahman Aldossary, Jiaru Bai, Shi Xuan Leong, Jorge Arturo Campos-Gonzalez-Angulo, Changhyeok Choi, Cher Tian Ser, Gary Tom, Andrew Wang, et al. El agente: An autonomous agent for quantum chemistry. *Matter*, 8(7), 2025.

A System Overview

In Table S1, a description of each agent, along with the LLM they are based on, can be found. Empirically, we found that most models performed significantly better when using gpt-5, compared to older models (gpt-4o, gpt-4.1).

Table S1: Overview of agents used in this work and models

Agent Name	Description	LLM Model
Supervisor	Responsible for understanding the user request, and developing a plan of actions needed to be performed to set up a simulation. Delegates to the various agents according to its plan.	gpt-5
Structure Expert	Finds the appropriate (placeholder) structure, and places a copy in the simulation folder.	gpt-5-mini
Force Field Expert	Given a request, decides what the appropriate force fields are. If necessary, it combines them, and writes new force field files (e.g., `force_field.def`, `pseudo_atoms.def`)	gpt-5
Simulation Input Expert	Creates a `simulation.input` file, depending on the requirements of the simulation. Needs to decide which keywords are appropriate, and where to fill in numbers and to template.	gpt-5
Coding Expert	Writes code to replicate the template folder for each necessary run. Needs to understand how the simulation template is set up, and which fields need to be filled in and how.	gpt-5
Evaluator	Evaluates the task performance of each agent by inspecting files created during their execution and flags any potential mistakes it finds.	gpt-5
Paper Search Agent	Uses Semantic Scholar search to find appropriate research papers, and downloads them.	gpt-5-mini
Paper Extraction Agent	Reads downloaded papers and extracts any relevant information from them (e.g., molecule definitions, interaction parameters).	gpt-5-mini
Force Field Writer	Reads the findings produced by the paper extraction agent and transforms them into RASPA force field files.	gpt-5

An overview of the tools can be found in Table S2. In addition to the tools enumerated here, agents have access to various tools for reading, writing, and copying files.

Table S2: Overview of tools available to various agents.

Tool Name	Description	Paramaters
list_example_simulation_inputs	Gives the names and description of example input files from the RASPA manual	-
read_atoms_in_file	Returns the set of atoms present in a `framework.cif` or `molecule.def` file.	file path
count_atom_type_in_cif	Counts how often a given atom type occurs in a CIF file.	file path, atom type
get_unit_cell_size	Returns the lattice parameters of the unit cell defined in a CIF file.	file path
get_all_force_field_descriptions	Lists the available force fields and their metadata.	-
get_atoms_in_ff_file	Lists the set of atoms for which parameters are defined in a force field file (`force_field.def`, `force_field_mixing_rules.def`, `pseudo_atoms.def`).	file path
semantic_scholar_search	Performs a search query using the Semantic Scholar.	query, limit, fields
download_paper	Downloads a paper given a DOI in the specified folder.	DOI, paper name
read_paper_headers	Lists the section headers of a paper after it has been parsed.	paper name
read_paper_section	Returns the content of the specified section (e.g., introduction) of a paper.	paper name, section

B Run Details

In Table S3, a more detailed explanation can be found on issues and mistakes during the simulation setup process. Overall, most mistakes are minor and could be fixed in a more robust, future version of the system.

Table S3: Notes on simulation setups with mistakes/intricacies

Task	Strucutre	Adsorbate	Notes
Isotherm	1	3	In multiple runs, all adsorbate files were copied into each simulation folder. Only the correct adsorbate was used in `simulation.input`, resulting in correct simulations.
HOA	500	1	In one of the runs, all possible moves were defined (with 0 probability, except widom insertions) for the adsorbate. In another run, no moves were specified for the adsorbate, resulting in an incorrect simulation where the adsorbate doesn't move.
HOA	500	3	In one of the runs, the structure CIF files were not copied, resulting in failed simulations. In multiple runs, redundant/unused files were left as part of the force field.
Isotherm	500	1	In one of the runs, a minimum amount of unit cells was enforced, resulting in many structures with more unit cells than necessary, resulting in slower simulations.
Isotherm	500	3	Rather than generating separate simulations for all three adsorbates, a mixture isotherm was calculated in one of the simulations. While this is a valid simulation, this was not requested in the task. In another run, a cutoff of 24 Å was selected, resulting in twice as many unit cells.

C Combined System Run

In Figures S1 and S2, a full trace is provided, to illustrate the systems behavior. For clarity, some messages have been summarized or omitted, highlighting the key interactions and decision points while omitting routine or repetitive exchanges.

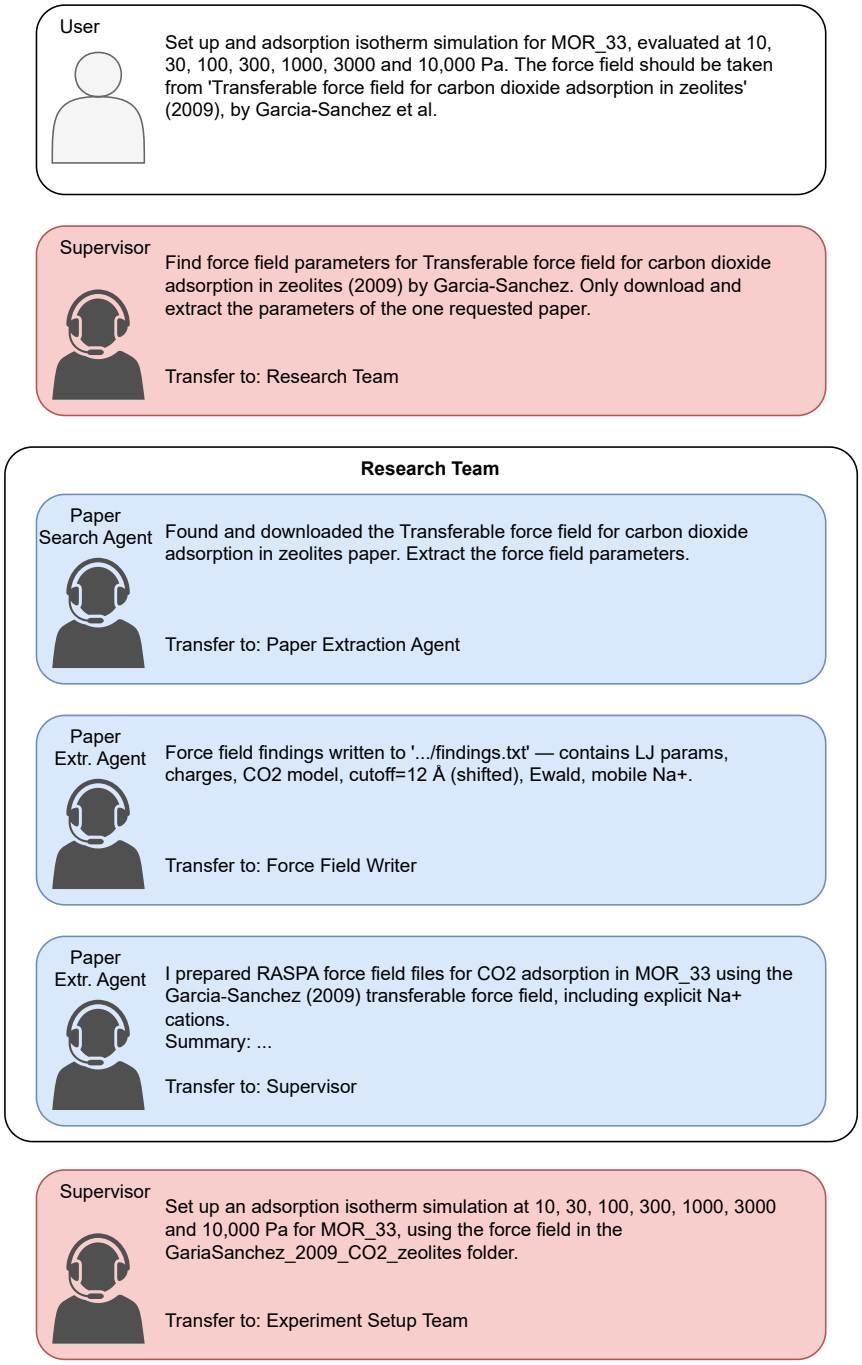

Figure S1: First part of the trace of the full system run.

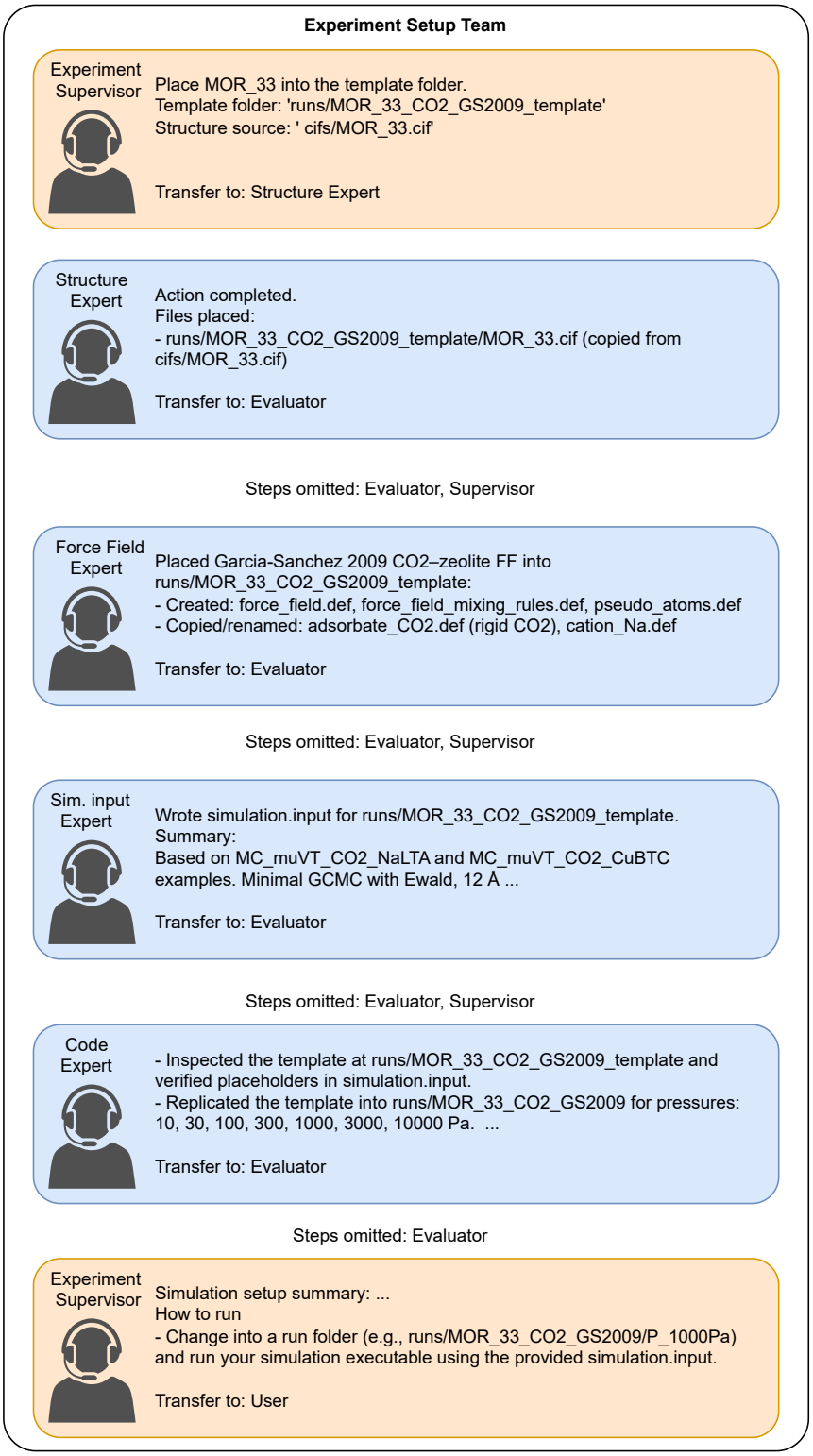

Figure S2: Second part of the trace of the full system run.