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(Henkel) **Henkel** ✔

Molecular dynamics modeling for predicting compound interactions

CHEMICALS

Background

Molecular Dynamics (MD) modeling is a powerful computational method used to simulate the physical movements of atoms and molecules over time, allowing researchers to observe molecular systems in action (at the nanoscale). This technique, combined with in silico screening, plays a crucial role in predicting the behavior and interactions of new chemistries.

While MD modeling enables virtual testing of compound efficacy, safety, and interactions, a significant challenge remains: ensuring that these models accurately reflect experimental observations. It is essential to develop MD models capable of verifying experimental results and calculating relevant parameters comparable to those observed in lab experiments. In the context of cosmetic and laundry detergent applications, these models could support product development by predicting viscosity changes upon incorporation of various small molecules, simulating film formation on hair or textile fibers, and anticipating phase behavior in surfactant-polymer mixtures.

Developing hybrid models that can combine calculated parameters from MD with trained artificial intelligence (AI) models could lead to improved predictive accuracy and

Submit Proposal

✔ Complete

⚡ **Easy Apply**

⬆ **Share**

Seeking partners focused on

Analytical Chemistry   Artificial Intelligence

Biochemistry   Bioinformatics

Biomolecular Processes   Biopharmaceutics

Biophysics   Biosystems   Cell Biology

Chemical Physics   39 more

Frequently Asked Questions

What are the proposal questions?

Where do I submit a proposal?

Who is eligible to submit a proposal?

provide the opportunity for high throughput screening prior to laboratory testing.

What we're looking for

We are looking for modeling solutions with strong predictive accuracy to identify new ingredients for cosmetic applications and/or laundry detergents. We are particularly interested in models that can predict interactions of compounds with hair, skin, or textile substrates and estimate core functionalities, such as film formation on hair or color retention on textiles. We are also open to models capable of predicting interactions within complex formulations, such as viscosity changes and the complexation of polymers and surfactants.

Solutions of interest include:

- Molecular dynamics techniques
- Hybrid modeling of MD and AI
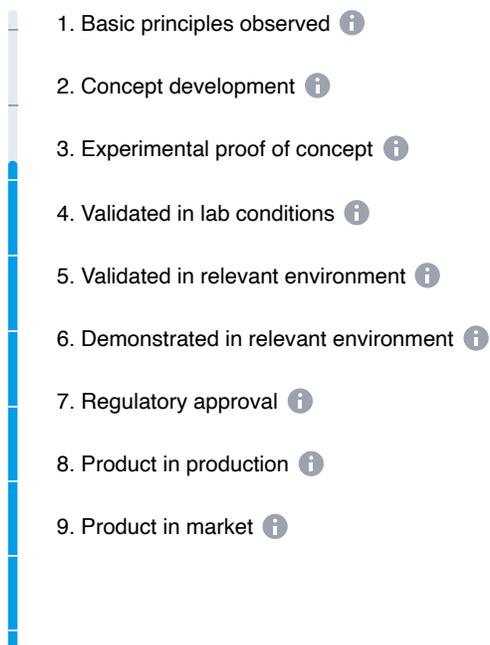
Our must-have requirements are:

- Proof of concept for any of the above-mentioned applications

Our nice-to-have's are:

- Uses open-source software like LAMMPS or GROMACS

Acceptable technology readiness levels (TRL):　　　Levels 3-9 ⓘ

1. Basic principles observed ⓘ
2. Concept development ⓘ
3. Experimental proof of concept ⓘ
4. Validated in lab conditions ⓘ
5. Validated in relevant environment ⓘ
6. Demonstrated in relevant environment ⓘ
7. Regulatory approval ⓘ
8. Product in production ⓘ
9. Product in market ⓘ

What we can offer you

Eligible partnership models:

Sponsored research   Co-development   Supply/purchase

Licensing   Equity investment

Benefits:

ⓢ Sponsored Research

Up to $50K for a proof-of-concept, with additional potential funding for further development of the project.

🧠 Expertise

Partners will have access to Henkel's domain expert knowledge within the context of the proof-of-concept.

🗄 Data

Necessary data for the validation of the developed model can be provided based on project requirements.

Who we are

Bringing numerous product innovations to the market, like the first self-acting laundry detergent in the world, the first ever liquid hair shampoo and the first hair spray, just to name a few – we have shaped the lives of millions of people. Henkel looks back on a great history of innovations that revolutionized markets multiple times, and this tradition still continues to this day through continuous investments in research and development. Together with universities and other research institutes, the international research team at Henkel Consumer Brands is constantly developing innovative products to delight our customers and consumers and exceed their expectations.

Learn more

Reviewers

Shuqing Wang

Global R&D Manager Disruptive Innovation & Partnerships

Maria Trinchera

Head of Disruptive Innovation & Partnerships

Q&A with Henkel

The Q&A is now closed.

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Q. **What is the timescale? With $50k I could consider deploying a PD part-time (upto 50%) for a year to adapt the MD models we developed to simulate hair/skin keratin binding and skin lipid partition for the project needs**

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GL Guoping Lian, Principal Investigator, University of Surrey

December 13, 2024

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