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DC2: Theory of identification, selection and evolution of autocatalytic network

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Host institution: Parmenides Foundation (PARM), Center for the Conceptional Foundations of Science, Pöcking, Germany



We are an international group interested in the evolution of systems at various levels from chemistry to language. Although the core activity is theoretical, collaboration with experimental groups is important and encouraged. We have an eminent past in the theory of evolution, minimal life-like chemical (super)systems, replicator theory, and multilevel selection, including replicators in protocells. The Parmenides Foundation provides a diverse and high-level intellectual environment and is a smoothly running organisation. The cohabiting Paradigmatic Innovations GmbH grew out from the same intellectual roots, and provides tools for state-of-the-art knowledge representation and strategic reasoning.

Project description: Identification of autocatalytic parts in computationally generated large chemical networks and assessment of their evolutionary potential in "naked" and compartmentalised form. DC2 will: (1) Generate large chemical networks and assign kinetic rate constants using AI algorithms. (2) Analyse the chemical networks to (a) identify autocatalytic subnetworks (ASN), (b) check that they are capable of exponential growth, (c) measure the prevalence of ASNs and (d) predict by AI the expected density of ASNs. (3) Use stochastic kinetics to follow how primitive starting compounds populate the network by chemical reactions. (4) Look for "ecological" interactions between ASNs.

Secondments: This project is carried out in strong collaboration with the following groups, and visits to their laboratories are expected during the project. A willingness to travel and spend time abroad is therefore essential:

- Host: École Supérieure de Physique et de Chimie Industrielles de la Ville de Paris (ESPCI) | Length: 2 months
 | Purpose: Characterisation of reproducing compartmentalised systems.
- Host: University of Groningen (RUG) | Length: 2 months | Purpose: Exchange between theoretical and experimental approaches.
- Host: Paradigmatic Innovations GmbH (PARA) | Length: 3 months | Purpose: Explore the option space for and representation of the results to be achieved by the most modern knowledge-representation methods.

Eligibility conditions:

 MSc in chemistry or computational/systems biology. Candidates with a background in computational or theoretical chemistry are especially encouraged to apply. DC2 will enrol in the <u>Doctoral Program of the</u> <u>Faculty of Chemistry and Pharmacy of LMU Munich</u>. Corresponding admission requirements apply.

Required Skills:

• Demonstrated skills in at least one relevant programming language and user-level understanding of linear algebra and differential equations. Creativity, intellectual risk-taking and interest in understanding of novel ideas. English as the working language, possibly complemented by some German.

Monthly allowances:

Living allowance: €3400*Mobility allowance: €600

Family allowance, if applicable: €660

Estimated gross salary: ~40,000 €/year

* The living allowance is adjusted by a <u>country correction coefficient</u>, depending on the country where the host institution is located. The exact net salary is dependent on local tax and social and health insurance regulations and will be confirmed upon appointment.

Enquiries

For general information about the DarChemDN visit the <u>project website</u> or send an email to <u>info@darchem-dn.eu</u>.



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How to apply

To complete your online application, visit the <u>DarChemDN recruitment web page</u>.

Required documents:

- Cover Letter
- Curriculum Vitae (including contact information of two referees)
- Copy of Transcripts
- Copy of Diplomas (if available at the time of application otherwise please provide a confirmation with the expected graduation date)

Only shortlisted applicants will be contacted. Interviews are expected to be online in November/December 2023.

Application deadline: To receive full consideration, applications must be submitted before 31 October 2023.