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Hybridising fundamental thermodynamic and graph neural network based models for the prediction of API solubility in mixed solvents

PhD (Chemical Engineering) OR MEng (Chemical Engineering) (Research)
(read more here about the programme and admission requirements)

Host: Prof. Jamie Cripwell

Commencement: The successful candidate must assume postgraduate work in January 2027.

Bursary: The successful candidate will be able to apply for an NRF project-linked bursary in 2027 **subject to successful funding of the wider project.**
Interested candidates are encouraged to contact the host for project details for the open NRF call ending 03 July 2026.

Solubility is an important property in both the synthesis/separation of active pharmaceutical ingredients (APIs) as well as for their efficacy in the human body. Decades of largely heuristic experimental measurements have culminated in large databases of pure solvent solubility data, which itself has provided the foundation for highly accurate machine learning models that can predict solubility based on API features. However, this success does not extrapolate to mixed solvents given the comparative lack of solubility data in such systems. This is inherently a thermodynamic problem – specifically, solid-liquid equilibria – which can be well described by state-of-the-art thermodynamic models. The proposed study will investigate ways of hybridising these modelling paradigms for improved and generalisable predictions in mixed solvents.

The project falls under the *SECrET: Solvent Engineering for API Crystallization Experiments leveraging predictive Thermodynamics and machine learning* project, submitted for funding under the SA-Flanders (FWO) Collaborative Research Projects funding instrument of the NRF as a collaboration with KU Leuven in Belgium and Sefako Makgatho Health Sciences University. **The outcome of this funding application will only be confirmed in December 2026, but projects kick off in 2027.**

The position is for full time on-campus studies only.

Requirements

- **For PhD applicants:** A master's degree (MEng/MSc or similar) in chemical engineering or related field from an accredited tertiary institution.
- **For MEng applicants:** A bachelor's degree (BEng/BScEng or similar) in chemical engineering from an accredited tertiary institution. Applicants with a BSc Honours degree in Chemistry or Pharmaceutical Science will also be considered. *Note that applicants with BTech, National Diploma, or Advanced Diploma qualifications will not be considered for these positions.*
- Applicants must display academic excellence (**minimum** requirement is an average of >65% in the final year of the previous degree).
- Previous experience in open-source coding languages (in particular Julia and scientific computing with Python) is a requirement for the project. A record of coding experience or projects (e.g. GitHub repositories) will be a definite advantage.
- Preference will be given to South African citizens and permanent residents who display academic excellence.

Application

Interested candidates must provide a cover letter, CV, degree certificate(s), complete academic transcript(s) (and Masters thesis, in the case of PhD applicants) and contact details of at least three academic references. Applicants may also send their final-year research project (or similar) for an example of previous academic written work. Incomplete applications will not be considered. Applications can be sent to cripwell@sun.ac.za. Candidates may consider their application unsuccessful if they do not receive any feedback within four weeks of applying.

Further to submitting the application documents to Prof Cripwell, candidates must also complete and submit an institutional application. Please read more about the application process here.

Stellenbosch University reserves the right not to fill the position.