Domain-Specific Language (DSL) for Nanomaterial Representation

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1. Introduction

Nanoinformatics can benefit from standardized nanomaterial representations to depict the unique complexity and variety of possible nanoforms and their dynamic nature. This work introduces a new metalanguage designed as a domain-specific language (DSL) to address these challenges and support knowledge sharing. Our motivation stems from the limitations of existing NM representations, which struggle to encapsulate the vast diversity of NM compositions, sizes, shapes, surface chemistries, etc. and also address the nanoparticle dynamics.

2. Methodology

We employed a methodology centered around defining specific objectives crucial for the DSL's development, including the accurate portrayal of NMs' structural and morphological features without necessitating major future revisions. The DSL prototype is built upon the essential components identified in [1]. The language's specification, articulated in Backus-Naur Form (BNF), ensures a comprehensive and extensible schema, laying the foundation for detailed nanomaterial descriptions.

3. DSL Capabilities

Our proposal illustrates the DSL's capacity for nuanced representation, able to consider the distributions of NM composition, morphology, size etc., interfaces and hierarchical structuring, modifications, and the relationships among different NM entities. The proposed DSL provides a flexible implementation framework to describe relationships between different states of a NM and information on the transitions between those states, extending to the description of NM dynamics, evolution and interactions.

4. Discussion

The discussion highlights the DSL's potential to advance nanomaterial documentation, offering significant advancements over conventional representation systems, by enhancing data management and query capabilities, and providing a robust framework for representing both fundamental and complex aspects of nanomaterials. This is crucial since NMs are rarely found in their pristine (i.e., as synthesized) forms and they constantly evolve through interactions and through their integration with biofluids, the

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environment etc. Poor consideration of these dynamic phenomena may reduce the accuracy of predictive nanoinformatics models [2].

5. Conclusions

This work aims to initiate a discussion for a collaboration to develop and implement a standard representation able to capture the real particle dynamics using the proposed DSL-based approach.

6. References

[1] Blekos, K., Chairetakis, K., Lynch, I., & Marcoulaki, E. (2023). Principles and requirements for nanomaterial representations to facilitate machine processing and cooperation with nanoinformatics tools. Journal of Cheminformatics, 15(1), 44.

[2] Wyrzykowska, E., Mikolajczyk, A., Lynch, I., Jeliazkova, N., Kochev, N., Sarimveis, H., ... & Puzyn, T. (2022). Representing and describing nanomaterials in predictive nanoinformatics. Nature Nanotechnology, 17(9), 924-932.