NOMAD

NOVEL MATERIALS DISCOVERY

NOMAD Laboratory Centre of Excellence

Industry Interview - Dr. Michael Krein (Lockheed Martin)

LOCKHEED MARTIN

Lockheed Martin is "a global security and aerospace company that employs approximately 125,000 people worldwide and is principally engaged in the research, design, development, manufacture, integration and sustainment of advanced technology systems, products and services". Their mission is to solve complex challenges, with the aim of delivering innovative solutions to help customers worldwide keep people safe, and provide essential services. A central goal is to advance scientific discovery.

Dr. Krein noted that **industry currently prefer to rely on proprietary data**, such as historical manufacturing data, or on verified/certified third party data made available by specialized companies. To date, there is a lack of confidence in free open source data, which we need to address by starting to build a trust chain. Companies could internally validate open data, adding value at little cost. In-house data validation requires assessing the data 'pedigree', ensuring t**raceability and reproducibility**, which NOMAD could enable by providing a set of information for each data entry, namely: code versioning, input files and possibly a reference. Further confidence could be achieved by performing random checks, e.g., double-checking some open source results by re-doing the chosen set of calculations.

We discussed in detail how NOMAD could improve how industry accesses, uses and exploits materials data in the medium term. Dr. Krein noted that **Intellectual property issues** are likely to arise, but that NOMAD has already addressed many potential obstacles to transparent free usage (e.g., NOMAD user activity will not be tracked). The size of the NoMaD Repository, which is constantly growing, was identified as another potential obstacle as the database could get too large to be easily explored/accessed. However, this could be the **basis for an 'industry case study'**. Dr. Krein suggested that NOMAD could position itself within the ICME (integrated computational materials engineering) workflow, a simulation (data)-heavy approach that was initiated by Ford (screening of aluminum alloys and processes). The NOMAD database could be an ideal platform for implementing high throughput screening, perhaps starting from applications more related to the active device realm (e.g., solar cell development, thermoelectricity). Dr. Krein noted that potential case studies should not be geared/expected to address or immediately impact *current* industry developments. In fact, NOMAD should act at a higher level, and focus on providing some analysis examples meant to showcase its potential and possibly to trigger seminal ideas strategically useful from an industry user perspective.

To drive NOMAD interactions with industry forward, Dr. Krein stressed the **importance of effective two-way communications**. He recommended preparing a brochure, organizing industry workshops and enabling interactive Q&A sessions with developers as software tools become available. Webinars and other modern form of communications/training are also conceivable, to introduce NOMAD and its potential benefits to our target industries. Engagement with individual industry representatives who use materials data in their day-to-day work was recommended, facilitated by presentation of example cases, tutorials, and informational material that could be included on NOMAD's website.

In closing, Dr. Krein noted that the materials modelling community has played too limited a role in the rapid growth of science and technology in the past 20-30 years, considering its potential. NOMAD could help to improve on this, and be an ideal platform to raise awareness of materials modelling advances and improve the perception of modelling data by private sector researchers/engineers.

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