Feasible Atomistic Simulations for the fusion project at ANL

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- **Argonne National Laboratory was a place where Molecular Dynamics method was born (1964) and we are planning to turn it to a Center of Molecular Dynamics Excellence (CMDE) – 200?**

- **New CMDE areas will include Classical & Quantum: MD, MC, ART**

The Enigma and Power of MD

• **Isaac Newton**	**1687**
• **Alder and Wainwright** **(MD of hard spheres)**	**1957, 1959**
• **Rahman** **(MD of liquid Argon)**	**1964, Argonne Nat. Lab**
• **Rahman, Stillinger** (MD of water)	**1974, Argonne Nat. Lab**
• **Rahman, Parrinello** (MD of crystals)	**1980, Argonne Nat. Lab**

MD Codes are simple and freely downloadable;
However, the data are excessive ➔ Avogadro Number;
As MD gives raw data ➔ the Analysis is more important;
The Enigma and Power of MD is in Theoretical Physics Analysis

Gallium & Tin Targets

- **Helium and Hydrogen bubble formation and surface coverage in liquid Ga, Sn;**
- **Retention coefficients of liquid Ga, Sn targets irradiated with low energy ions;**
- **Sputtering coefficients of liquid Ga, Sn targets irradiated with low energy ions;**
- **Reflection coefficients of liquid Ga, Sn targets with the above mentioned ions.**

Alloy (Li, Ga, Sn Etc) Targets

- **Engineering a suitbale alloy consisting of many liquid metals, in order to achieve the desired features;**
- **Sputtering of Liquid Alloy targets with low energy Helium and Hydrogen ions;**
- **Reflection and retention coefficients of liquid alloy targets with low energy Helium and Hydrogen ions.**