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Lost in Terabytes of Simulations or Experiments? NOMAD can FAIRify the Chaos

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High-throughput simulations and data-intensive experimental measurements are now central to many branches of physics, from predicting materials to benchmarking force-field models and training machine-learning potentials. Modern studies can generate terabytes of heterogeneous output files, yet much of this valuable information remains locked inside program-specific log files, instrument formats, and binary blobs. The absence of a common, machine-readable description hinders reproducibility, slows cross-code comparison, and ultimately limits scientific reach.

The open-source **NOMAD** platform (nomad-lab.eu), developed within the German NFDI consortium **FAIRmat**, tackles this bottleneck by implementing the **FAIR** data principles **(Findable, Accessible, Interoperable, Re-usable)** for computational and experimental materials science.[1,2] Its plugin-based architecture lets researchers attach custom parsers, metadata schemas, and visualization widgets to a wide range of electronic-structure codes—Gaussian, VASP, FHI-aims, ORCA, and more—and to experimental techniques such as X-ray diffraction or photoelectron spectroscopy, transforming disparate outputs into a coherent, queryable database. Integrated notebooks, APIs, and workflow functionalities then make the curated data immediately available for statistical analyses, surrogate-model construction, or AI-driven discovery.

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