

## Supplementary Information

# Developments and applications of the OPTIMADE API for materials discovery, design, and data exchange

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PROVIDER	N <sub>1</sub>	N <sub>2</sub>	N <sub>3</sub>	N <sub>tot</sub>
AFLOW	704,302 (700,192)	63,017 (62,293)	413,797 (382,554)	3,530,330
Alexandria*	939,084	48,510	437,768	5,055,842
COD	458,249 (416,314)	4,082 (3,896)	34,739 (32,420)	512,282
CMR	2,811	386	0	16,789
JARVIS-DFT	9,017	1,426	8,084	77,096
Materials Cloud*	961,564	4,218	136,176	4,515,120
Materials Project	34,424 (27,309)	3,750 (3,545)	11,861 (10,501)	154,387
MPDD	811,136	80,195	490,900	3,975,666
MPOD	91	8	16	401
MPDS	-	-	-	507,178
NOMAD	4,451,056 (3,359,594)	587,923 (532,123)	2,092,989 (1,611,302)	12,116,021
odbx*	125,648 (55)	3,179 (54)	17,009 (0)	523,216
omdb	58,718 (58,718)	690 (690)	7,428 (7,428)	68,566
OQMD	261,400 (153,113)	15,375 (11,011)	81,673 (70,252)	1,226,781
TCOD	7,161 (2,631)	296 (296)	662 (660)	7,452
2DMatpedia	1,172	739	255	6,351

Table 1. The table from Ref.<sup>1</sup> recreated in March 2024, with new providers. The final column indicates the total number of structures served by each OPTIMADE API. Providers that serve multiple databases are indicated with \*. Results for Materials Cloud and Materials Cloud Archive have been aggregated under the same title. The corresponding values from the 2021 paper<sup>1</sup> are provided in brackets, where appropriate.

## References

- 1 C. W. Andersen et al. OPTIMADE: an API for exchanging materials data. *Scientific Data*, 8:217, 2021. DOI: [10.1038/s41597-021-00974-z](https://doi.org/10.1038/s41597-021-00974-z).