# Search for ambient superconductivity in the Lu-N-H system

**L. Boeri**

*Physics Department, Sapienza Università di Roma, Italy*

Recently, Dasenbrock et al. reported room-temperature superconductivity at near-ambient pressure in N-doped lutetium hydride [1], stimulating a heated debate on the reproducibility of their results.[2] In the absence of conclusive experimental information on the nature and composition of the superconducting phase, first-principles crystal structure prediction represents an invaluable tool to explore the phase diagram and identify candidate phases that could explain the observed superconductivity. [3]

In this work we performed a comprehensive, detailed study of the phase diagram of the Lu-N-H system, sampling over 200,000 different structures to search for superconducting phases. Out of the more than 150 structures predicted to be metastable within ~ 50 meV from the convex hull we identify 52 viable candidates for conventional superconductivity, for which we computed their superconducting properties from Density Functional Perturbation Theory. Although for some of these structures we do predict a finite superconducting $T_c$, none is even remotely compatible with room-temperature superconductivity reported by Dasenbrock-Gammon et al. [4] Our results are in agreement with other studies that employ different methods for crystal structure prediction, which also conclude that room or even high-temperature superconductivity within the conventional electron-phonon scenario is extremely unlikely in the Lu-N-H system. [5]

[1] N. Dasenbrock-Gammon et al., Nature **615** , 244 (2023).
[2] *see for example:* X. Ming et al., Nature 2023, and N. P. Salke et al., cond-mat/2306.06301.
[3] J.A. Flores-Livas et al., Physics Reports **856**, 1-78 (2020).
[4] P.P. Ferreira et al., cond-mat/2304.04447.
[5] M. Liu et al, cond-mat/2303.06554; K.P. Hilleke et al., cond-mat/2303.15622; M. Gubler et al., cond-mat/2306.07746.