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        https://doi.org/10.1038/s41586-023- 06792-0 10 Liu, Y.; Checa, M.; Vasudevan, R. K.
        Synergizing human expertise and AI efficiency with language model for microscopy
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        5, 02LT01 (2024). https://doi.org/10.1088/2632- 2153/ad52e9 11 Gao, Y.; Xiong, Y.;
        Gao, X.; Jia, K.; Pan, J.; Bi, Y.; Dai, Y.; Sun, J.; Wang, H.; Wang, H. Retrieval-
        augmented generation for large language models: A survey. arXiv preprint
        arXiv:2312.10997 2 (2023). 12 Ke, Y. H.; Jin, L.; Elangovan, K.; Abdullah, H. R.;
        Liu, N.; Sia, A. T. H.; Soh, C. R.; Tung, J. Y. M.; Ong, J. C. L.; Kuo, C.-F.; Wu,
        S.-C.; Kovacheva, V. P.; Ting, D. S. W. Retrieval augmented generation for 10 large
        language models and its generalizability in assessing medical fitness. npj Digital
        Medicine 8, 187 (2025). https://doi.org/10.1038/s41746-025- 01519-z 13 Young, S. R.;
        Maksov, A.; Ziatdinov, M.; Cao, Y.; Burch, M.; Balachandran, J.; Li, L.; Somnath, S.;
        Patton, R. M.; Kalinin, S. V.; Vasudevan, R. K. Data mining for better material
        synthesis: The case of pulsed laser deposition of complex oxides. Journal of Applied
        Physics 123, 115303 (2018). https://doi.org/10.1063/1.5009942 14 Lu, M.; Ji, H.;
        Zhao, Y.; Chen, Y.; Tao, J.; Ou, Y.; Wang, Y.; Huang, Y.; Wang, J.; Hao, G. Machine
        Learning-Assisted Synthesis of Two-Dimensional Materials. ACS Applied Materials &
        Interfaces 15, 1871-1878 (2023). https://doi.org/10.1021/acsami.2c18167 15 Snapp, K.
        L.; Verdier, B.; Gongora, A. E.; Silverman, S.; Adesiji, A. D.; Morgan, E. F.;
        Lawton, T. J.; Whiting, E.; Brown, K. A. Superlative mechanical energy absorbing
        efficiency discovered through self-driving lab-human partnership. Nature
        Communications 15, 4290 (2024). https://doi.org/10.1038/s41467-024-48534-4 22 16
        Park, B.-I.; Kim, J.; Lu, K.; Zhang, X.; Lee, S.; Suh, J. M.; Kim, D.-H.; Kim, H.;
        Kim, J. Remote Epitaxy: Fundamentals, Challenges, and Opportunities. Nano Letters 24,
        2939- 2952 (2024). https://doi.org/10.1021/acs.nanolett.3c04465 17 Haque, A.; Mandal,
        S. K.; Parate, S. K.; D'souza, H. J.; Nukala, P.; Raghavan, S. Free standing
        epitaxial oxides through remote epitaxy: the role of the evolving graphene
        microstructure. Nanoscale 17, 2020-2031 (2025). https://doi.org/10.1039/D4NR03356F 18
        Wohlgemuth, M. A.; Trstenjak, U.; Sarantopoulos, A.; Gunkel, F.; Dittmann, R. Control
        of growth kinetics during remote epitaxy of complex oxides on graphene by pulsed
        laser deposition. APL Materials 12 (2024). https://doi.org/10.1063/5.0180001 19
        Manzo, S.; Strohbeen, P. J.; Lim, Z. H.; Saraswat, V.; Du, D.; Xu, S.; Pokharel, N.;
        Mawst, L. J.; Arnold, M. S.; Kawasaki, J. K. Pinhole-seeded lateral epitaxy and
        exfoliation of GaSb films on graphene-terminated surfaces. Nature Communications 13,
        4014 (2022). https://doi.org/10.1038/s41467-022-31610-y 20 Yoon, H.; Truttmann, T.
        K.; Liu, F.; Matthews, B. E.; Choo, S.; Su, Q.; Saraswat, V.; Manzo, S.; Arnold, M.
        S.; Bowden, M. E.; Kawasaki, J. K.; Koester, S. J.; Spurgeon, S. R.; Chambers, S. A.;
        Jalan, B. Freestanding epitaxial SrTiO3 nanomembranes via remote epitaxy using hybrid
        molecular beam epitaxy. Science Advances 8, eadd5328 (2022).
        https://doi.org/10.1126/sciadv.add5328 21 Kong, W.; Li, H.; Qiao, K.; Kim, Y.; Lee,
        K.; Nie, Y.; Lee, D.; Osadchy, T.; Molnar, R. J.; Gaskill, D. K.; Myers-Ward, R. L.;
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