

## PUBLICATIONS (Metrics from Google Scholar: 93 citations, h-index=4)

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### In production

- [13] BerkeleyGW-4.x: A portable exascale-ready software package for electronic excited-state properties of materials. M. Del Ben, Z. Li, F. H. da Jornada, D. Y. Qiu, D. A. Strubbe, D. Vigil-Fowler, A. Altman, B. A. Barker, A. Cepelloti, A. Chamapagne, Y. Chan, M. R. Filip, S. Gant, **R. R. Del Grande**, J. Harber, C. Hu, W. Huhn, O. Hull, W. Kim, M. H. Naik, C. S. Ong, S. Rafaely-Abramson, J. Ruan, W. Tang, P. Thomas, D. Weinberg, M. Wu, F. Zhao, F. Zhang, J. B. Neaton, J. R. Deslippe and S. G. Louie
- [12] Consequences of H  $sp^3$  doping in the electronic and optical properties of Carbon Nanotubes. **R. R. Del Grande**, M. G. Menezes, R. B. Capaz
- [11] Revisiting excited state forces from many-body Green's function formalism: approximations and benchmark. **R. R. Del Grande**, D. A. Strubbe. <https://doi.org/10.48550/arXiv.2502.05144>
- [10] How to choose efficiently the size of the Bethe-Salpeter Equation Hamiltonian for accurate exciton calculations on supecells. **R. R. Del Grande**, D. A. Strubbe. <https://doi.org/10.48550/arXiv.2502.19396>
- [9] Ab initio excited state forces from many-body Green's function formalism: relaxation of excited states and coherent phonon production. **R. R. Del Grande**, D. A. Strubbe
- [8] Assessing the accuracy of vibrations in the GAP machine learning potential for hydrogenated amorphous silicon. N. E. Simons, **R. R. Del Grande**, D. A. Strubbe

### Published

- [7] Flat bands and gaps in twisted double trilayer graphene. F. J. Culchac, **R. R. Del Grande**, M. G. Menezes, R. B. Capaz. Physical Review B, 111, 075111 (2025) <https://doi.org/10.1103/PhysRevB.111.075111>
- [6] Home experiments: a hands-on adaptation of the Experimental Physics II course at UFRJ for remote teaching. A. R. Hernández, A. M. Gomes, E. H.C.P. Sinnecker, **R. R. Del Grande**, R. B. Capaz and S. C. Cardoso. Rev. Bras. Ensino Fís. 43 (2021) <https://doi.org/10.1590/1806-9126-RBEF-2021-0248> (in Portuguese) (5 citations)
- [5] Flat bands and gaps in twisted double bilayer graphene. F. J. Culchac, **R. R. Del Grande**, R. B. Capaz, L. Chico, E. S. Morell. Nanoscale 12, 5014-5020 (2020) <https://doi.org/10.1039/C9NR10830K> (54 citations)
- [4] Energy barriers for collapsing large-diameter carbon nanotubes. **R. R. Del Grande**, A. F. Fonseca and R. B. Capaz. Carbon 159 161-165 (2020) <https://doi.org/10.1016/j.carbon.2019.12.030> (10 citations)
- [3] Layer breathing and shear modes in multilayer graphene: a DFT-vdW study. **R. R. Del Grande**, M. G. Menezes and R. B. Capaz J. Phys.: Cond. Matter 31 295301 (2019) <https://doi.org/10.1088/1361-648X/ab1995> (9 citations)
- [2] From Nanoscale Wetting Towards Enhanced Oil Recovery. R. Giro, M. B. Steiner, P. W. Bryant, **R. R. Del Grande**, M. Engel. Offshore Technology Conference Brasil - 27-29 (2015) <https://doi.org/10.4043/26232-MS> (4 citations)
- [1] Multi-scale modeling of wetting: effects of surface roughness. R. Giro, P. W. Bryant, M. B. Steiner, **Rafael R. Del Grande**, C. Feger, M. Engel. CILAMCE 2014 - XXXV Iberian Latin American Congress on Computational Methods in Engineering (2014) (1 citation)