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The converse approach to NMR chemical shifts from first-principles: application to finite and infinite aromatic compounds T. THONHAUSER, Wake Forest University, D. CERESOLI, N. MARZARI, MIT — We present first-principles, density-functional theory calculations of the NMR chemical shifts for polycyclic aromatic hydrocarbons, starting with benzene and increasing sizes up to the one- and two-dimensional infinite limits of graphene ribbons and sheets. Our calculations are performed using a combination of the recently developed theory of orbital magnetization in solids, and a novel approach to NMR calculations where chemical shifts are obtained from the derivative of the orbital magnetization with respect to a microscopic, localized magnetic dipole. Using these methods we study on equal footing the ^{1}H and ^{13}C shifts in benzene, pyrene, coronene, in naphthalene, anthracene, naphthacene, and pentacene, and finally in graphene, graphite, and an infinite graphene ribbon. Our results show very good agreement with experiments and allow us to characterize the trends for the chemical shifts as a function of system size.

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