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Sommario/riassunto	This thesis demonstrates the value of theoretical approaches in the

discovery of new superconducting materials. It reports a detailed study of the recently discovered nickel-oxide (nickelate) superconductors using multiple first-principles computational tools, from density functional theory to dynamical mean field theory. In the context of superconductivity, discoveries have generally been linked to serendipitous experimental discovery; this thesis reports some of the few examples of predictions of new superconductors that have later been realized in practice, a prime example of the significance of the methodology it expounds. Overall, it represents a seminal systematic work in the electronic structure theory of the emergent field of nickelate superconductivity.