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Altri autori (Persone)	StoltzGabriel RoussetMathias <1980->
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Sommario/riassunto	This monograph provides a general introduction to advanced computational methods for free energy calculations, from the systematic and rigorous point of view of applied mathematics. Free energy calculations in molecular dynamics have become an outstanding and increasingly broad computational field in physics, chemistry and molecular biology within the past few years, by making possible the analysis of complex molecular systems. This work proposes a new, general and rigorous presentation, intended both for practitioners interested in a mathematical treatment, and for applied mathematicians inte