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### DESCRIPTION

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*Computational and Theoretical Chemistry* publishes high quality, original reports of significance in **computational** and theoretical **chemistry** including those that deal with problems of structure, properties, energetics, weak interactions, reaction mechanisms, catalysis, and reaction rates involving atoms, molecules, clusters, surfaces, and bulk matter. Reports on new algorithms and comprehensive assessments of existing ones, and applications to new types of problems are especially welcome. Manuscripts that apply standard methods to specific chemical problems and/or to specific molecules are appropriate if they report novel results for an important problem of high interest and/or if they are used to develop significant new insights.

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