Stress-tensor Calculations in the All-electron Full-potential Linearized Augmented Plane Wave method

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Efficient stress-tensor formulation has been available for some decades in first-principles calculations with the pseudo-potential plane-wave methods. Although stress formulation in the full-potential linearized augmented plane wave (FLAPW) method was proposed by Thonhauser *et al*. in 2002, they reported only the results for Al and Si [1]. We reformulated stress-tensor calculation in the FLAPW method based on the Soler-Williams basis [2] within the local density and generalized gradient approximations and performed comprehensive tests of the formulation not only for Al and Si but also for several material systems [3]. Through the tests, we confirmed that stress tensors were precisely evaluated by using our proposed formulation.

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