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Bibliography


[45] Nicholas Metropolis, Arianna W. Rosenbluth, Marshall N. Rosenbluth, Augusta H. Teller, and Edward Teller (1953), “Equation of State Calculations by Fast Computing Machines,” Journal of Chemical Physics. The previous link is to the Americaian Institute of Physics and if you do not have access to Science Sitations you may not be able to retrieve this paper.


