

	Publication	# cites	Title	Author(s)
1	PRB (1988)	30198	Development of the Colle-Salvetti Correlation-Energy into a Functional of the Electron-Density	Lee, CT; Yang, WT; Parr, RG
2	PRA (1988)	18610	Density-Functional Exchange-Energy Approximation with Correct Asymptotic-Behavior	Becke, AD
3	PR (1965)	17196	Self-Consistent Equations Including Exchange and Correlation Effects	Kohn, W; Sham, LJ
4	PRL (1996)	15663	Generalized Gradient Approximation Made Simple	Perdew, JP; Burke, K; Ernzerhof, M
5	PRB (1976)	9063	Special Points for Brillouin-Zone Integrations	Monkhorst HJ; Pack JD
6	PRB (1996)	8652	Efficient Iterative Schemes for Ab Initio Total-Energy Calculations Using a Plane-Wave Basis Set	Kresse, G; Furthmuller, J
7	PRB (1992)	8421	Accurate and Simple Analytic Representation of the Electron-Gas Correlation-Energy	Perdew, JP; Wang, Y
8	PRB (1981)	8307	Self-Interaction Correction to Density-Functional Approximations for Many-Electron Systems	Perdew, JP; Zunger, A
9	PR (1934)	8272	Note on an Approximation Treatment for Many-Electron Systems	Moller, C; Plesset, MS
10	PRB (1986)	8013	Density-Functional Approx. for the Correlation-Energy of the Inhomogeneous Electron Gas	Perdew, J
11	PRB (1992)	7819	Atoms, Molecules, Solids, and Surfaces-Applications of the Generalized Gradient Approx. [...]	Perdew, JP; Chevary, JA; Vosko, SH; ...
12	PRB (1990)	7768	Soft Self-Consistent Pseudopotentials in a Generalized Eigenvalue Formalism	Vanderbilt, D
13	PRB (1964)	7594	Inhomogeneous Electron Gas	Hohenberg, P; Kohn, W
14	PRL (1980)	6645	Ground-State of the Electron-Gas by a Stochastic Method	Ceperley, DM; Alder, BJ
15	PRL (1986)	6517	Atomic Force Microscope	Binnig, G; Quate, CF; Gerber, C
16	PRL (1987)	6457	Inhibited Spontaneous Emission in Solid-State Physics and Electronics	Yablonovitch, E
17	PRB (1991)	5887	Efficient Pseudopotentials for Plane-Wave Calculations	Troullier, N; Martins, JL
18	PRB (1999)	5868	From Ultrasoft Pseudopotentials to the Projector Augmented-Wave Method	Kresse, G; Joubert, D
19	PR (1961)	5816	Effects of Configuration Interaction on Intensities and Phase Shifts	Fano, U
20	PR (1957)	5760	Theory of Superconductivity	Bardeen, J; Cooper, LN; Schrieffer, JR

Most cited papers in the history of the American Physical Society (from 1893 onwards – Physical Review, Physical Review Letters, Physical Review A/B/C/D/E, Review of Modern Physics; Marzari and Scheffler, February 2011). Those in boldface (1-14, 17 and 18) are on quantum simulations.