First principles calculations of La$_2$CuO$_4$ ANDREI PLAMADA, Institute for Theoretical Physics, ETH Zurich, ANTON KOZHEVNIKOV, Swiss National Supercomputer Centre, ETH Zurich, URS HAEHNER, MI JIANG, Institute for Theoretical Physics, ETH Zurich, PETER STAAR, IBM Research - Zurich, THOMAS MAIER, Computer Science and Mathematics Division and Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, THOMAS SCHULTHESS, Institute for Theoretical Physics, ETH Zurich — We use the DFT+DCA method for a high-end study of the electronic structure properties of La$_2$CuO$_4$. The parameters of a tight-binding model are created using the first-principles electronic structure calculations. The all-electron full-potential linearised augmented plane-wave method is used to solve the non-interacting band problem. Then the set of physically relevant Wannier functions is chosen as a basis for the underlying Hubbard model. The Wannier functions and the corresponding non-interacting Hamiltonian $H_{nm}^0(k)$ are created using the well-established downfolding approach. The screened Coulomb interaction parameters $U_{nm}$ of the model are computed using the constrained random-phase approximation technique. The double counting term is assumed to be a constant multiplied by the identity operator in the correlated subspace and it is determined based on first-principles considerations. The resulting \textit{ab-initio} parameterisation of the Hubbard model is solved within dynamical cluster approximation (DCA).