- 3	Density Matrix Minimization: Orthogonal Basis	
O	[XP. Li, R.W. Nunes, D. Vanderbilt, PRB 47, 10891 (193)]	
	Density matrix.	
	Let In> be the eigenstates of the Hamiltonian,	
	$\hat{H} n \rangle = \varepsilon_n n \rangle$	(1)
	Then the density matrix is defined as	
	$\widehat{\rho} = \sum_{n} n\rangle \Theta(\mu - \varepsilon_n) \langle n $	(2)
	(Idempotency: projection operator)	41 - 14 - 12 - 1
	$\widehat{\rho}^2 = \sum_{m} m\rangle \Theta(\mu - \varepsilon_m) \langle m \sum_{n} n\rangle \Theta(\mu - \varepsilon_n) \langle n $	
	$= \sum_{m,n} m\rangle \Theta(\mu - \varepsilon_m) \langle m n\rangle \Theta(\mu - \varepsilon_n) \langle n $ $= \sum_{m,n} m\rangle \Theta(\mu - \varepsilon_m) \langle m n\rangle \Theta(\mu - \varepsilon_n) \langle n $	
	$= \sum_{n} n\rangle \underbrace{\Theta^{2}(\mu - \varepsilon_{n})}_{= \Theta(\mu - \varepsilon_{n})} < n = \widehat{\rho}$	
	= O(µ-En)	
	$\therefore \hat{\rho}^2 = \hat{\rho}$	(3)
	(Normalization)	
	$T_n \hat{\rho} = \sum_{n} \langle n J \hat{\rho} n \rangle$	
	$= \sum_{n \mid m} \frac{\langle n \mid m \rangle}{\delta_{nm}} \frac{\partial \langle \mu - \varepsilon_{m} \rangle}{\delta_{mn}} \frac{\langle m \mid n \rangle}{\delta_{mn}}$	
	$= \sum_{n} \Theta(\mu - \varepsilon_n) = Ne$	127774
	$\therefore T_{\mathcal{R}} \hat{\rho} = \Sigma \Theta(\mu - \varepsilon_n) = N_e$	(4)
	where Ne is the number of electrons and μ is the cl	hemical
0	potential.	
	(Hermicity)	
	$\hat{\rho}^{\dagger} = \hat{\hat{\rho}}$	(5)

(Postive definiteness) All eigenvalues of $\hat{\rho}$ are 1 or 0; $\hat{\rho}$ is positive definite. Orthogonal representation Let { li> li=1,..., NM} be an orthonormal basis, <ili>=Sii, attached to atoms, where N is the number of atoms and M is the number of basis orbitals per atom. Pij = <iip ij> $= \sum_{n} \langle i | n \rangle \Theta(\mu - \varepsilon_n) \langle n | j \rangle$ $\frac{1}{\sqrt{n}} i \qquad \frac{1}{\sqrt{n}} i \qquad \frac{1}{\sqrt{n$ = $\sum_{n} \psi_{n,i} \Theta(\mu - \varepsilon_n) \psi_{j,n}^*$ (6)Grand-canonical energy: constrained minimization $\Omega = \text{tr}[\hat{\rho}(\hat{H}-\mu)]$ (X) $= \sum_{i,j} \rho_{ij} (H_{ji} - \mu \delta_{ji})$ (8) The ground state is obtained by minimizing Eq. (7) with the idempotency constraint, Eq. (3), for a given μ . The number of electrons for this ground state is then obtained from Eq. (4).

The modified grand potential is then defined as $\widetilde{\Omega} = \text{tr}[\widetilde{\rho}(\widehat{H} - \mu)] \qquad ($ $= \text{tr}[(3\widehat{\rho}^{2} \circ 2\widehat{\rho}^{3})(\widehat{H} - \widehat{\mu})] \qquad ($ $(\text{Gradient}) \qquad ($ $(\text{Gradient}) \qquad ($ $S\widetilde{\Omega} = \text{tr}[3(\widehat{\rho} \circ \widehat{\rho} + s\widehat{\rho}\widehat{\rho})(\widehat{H} - 2(\widehat{\rho}^{3} \circ \widehat{\rho} + \widehat{\rho} \circ \widehat{\rho} + s\widehat{\rho}\widehat{\rho}^{3})(\widehat{H} - \widehat{\mu})] \qquad ($ $= \text{tr}[3(\widehat{H}'\widehat{\rho} + \widehat{\rho} + \widehat{\mu})(\widehat{\rho} \circ \widehat{\rho} - 2(\widehat{H}'\widehat{\rho}^{3} + \widehat{\rho} + \widehat{\rho} + \widehat{\rho} \circ \widehat{H})(\widehat{\rho} \circ \widehat{\rho})] \qquad ($ $(\text{Outdie shifts}) \qquad ($ Note that the gradient is defined as $S\widetilde{\Omega} = \text{tr}(\frac{\Im \widetilde{\Omega}}{\Im \widehat{\rho}} \circ \widehat{\rho}) = \underbrace{\Sigma}_{ij} \begin{pmatrix} \Im \widetilde{\Omega} \\ \partial \widehat{\rho} \end{pmatrix}_{ij} \delta \widehat{\rho}_{ij} \qquad ($ $Comparing Egs. (14) and (15),$			
Let's defined a purified version of a trial density matrix, ρ , as $\tilde{\rho} = 3\hat{\rho}^2 - 2\hat{\rho}^3 \qquad ($ The modified grand potential is then defined as $\tilde{\Omega} = \text{tr}[\tilde{\rho}(\hat{H} - \mu)] \qquad ($ $= \text{tr}[(3\hat{\rho}^2 - 2\hat{\rho}^3)(\hat{H} - \hat{\mu})] \qquad ($ $\tilde{\Omega} = \text{tr}[(3(\hat{\rho} + \hat{\rho} + \hat{\rho} + \hat{\rho})(\hat{\rho} + \hat{\rho})(\hat{\rho})(\hat{\rho} + \hat{\rho})(\hat{\rho} + \hat{\rho})(\hat{\rho} + \hat{\rho})(\hat{\rho} + \hat{\rho})(\hat{\rho} + \hat{\rho})(\hat{\rho} + \hat{\rho})(\hat{\rho})(\hat{\rho} + $	_	- Unconstrained minimization	
The modified grand potential is then defined as $ \widetilde{Z} = \text{tr}[\widetilde{P}(\widehat{H} - \mu)] \qquad ($ $ = \text{tr}[(3\widehat{P}^{2} \cdot 2\widehat{P}^{3})(\widehat{H} - \widehat{\mu})] \qquad ($ $ = \text{tr}[(3\widehat{P}^{2} \cdot 2\widehat{P}^{3})(\widehat{H} - \widehat{\mu})] \qquad ($ $ = \text{tr}[(3\widehat{P}^{2} \cdot 2\widehat{P}^{3})(\widehat{H} - \widehat{\mu})] \qquad ($ $ = \text{tr}[(3\widehat{P}^{2} \cdot 2\widehat{P}^{3})(\widehat{H} - \widehat{\mu})] \qquad ($ $ = \text{tr}[(3\widehat{P}^{2} \cdot 2\widehat{P}^{3})(\widehat{H} - \widehat{\mu})] \qquad ($ $ = \text{tr}[(3\widehat{P}^{2} \cdot 2\widehat{P}^{3})(\widehat{H} - \widehat{\mu})] \qquad ($ $ = \text{tr}[(3\widehat{P}^{2} \cdot 2\widehat{P}^{3})(\widehat{H} - \widehat{\mu})] \qquad ($ $ = \text{tr}[(3\widehat{P}^{2} \cdot 2\widehat{P}^{3})(\widehat{H} - \widehat{\mu})] \qquad ($ $ = \text{tr}[(3\widehat{P}^{2} \cdot 2\widehat{P}^{3})(\widehat{H} - \widehat{\mu})] \qquad ($ $ = \text{tr}[(3\widehat{P}^{2} \cdot 2\widehat{P}^{3})(\widehat{H} - \widehat{\mu})] \qquad ($ $ = \text{tr}[(3\widehat{P}^{2} \cdot 2\widehat{P}^{3})(\widehat{H} - \widehat{\mu})] \qquad ($ $ = \text{tr}[(3\widehat{P}^{2} \cdot 2\widehat{P}^{3})(\widehat{H} - \widehat{\mu})] \qquad ($ $ = \text{tr}[(3\widehat{P}^{2} \cdot 2\widehat{P}^{3})(\widehat{H} - \widehat{\mu})] \qquad ($ $ = \text{tr}[(3\widehat{P}^{2} \cdot 2\widehat{P}^{3})(\widehat{H} - \widehat{\mu})] \qquad ($ $ = \text{tr}[(3\widehat{P}^{2} \cdot 2\widehat{P}^{3})(\widehat{H} - \widehat{\mu})] \qquad ($ $ = \text{tr}[(3\widehat{P}^{2} \cdot 2\widehat{P}^{3})(\widehat{H} - \widehat{\mu})] \qquad ($ $ = \text{tr}[(3\widehat{P}^{2} \cdot 2\widehat{P}^{3})(\widehat{H} - \widehat{\mu})] \qquad ($ $ = \text{tr}[(3\widehat{P}^{2} \cdot 2\widehat{P}^{3})(\widehat{H} - \widehat{\mu})] \qquad ($ $ = \text{tr}[(3\widehat{P}^{2} \cdot 2\widehat{P}^{3})(\widehat{H} - \widehat{\mu})] \qquad ($ $ = \text{tr}[(3\widehat{P}^{2} \cdot 2\widehat{P}^{3})(\widehat{H} - \widehat{\mu})] \qquad ($ $ = \text{tr}[(3\widehat{P}^{2} \cdot 2\widehat{P}^{3})(\widehat{H} - \widehat{\mu})] \qquad ($ $ = \text{tr}[(3\widehat{P}^{2} \cdot 2\widehat{P}^{3})(\widehat{H} - \widehat{\mu})] \qquad ($ $ = \text{tr}[(3\widehat{P}^{2} \cdot 2\widehat{P}^{3})(\widehat{H} - \widehat{\mu})] \qquad ($ $ = \text{tr}[(3\widehat{P}^{2} \cdot 2\widehat{P}^{3})(\widehat{H} - \widehat{\mu})] \qquad ($ $ = \text{tr}[(3\widehat{P}^{2} \cdot 2\widehat{P}^{3})(\widehat{H} - \widehat{\mu})] \qquad ($ $ = \text{tr}[(3\widehat{P}^{2} \cdot 2\widehat{P}^{3})(\widehat{H} - \widehat{\mu})] \qquad ($ $ = \text{tr}[(3\widehat{P}^{2} \cdot 2\widehat{P}^{3})(\widehat{H} - \widehat{\mu})] \qquad ($ $ = \text{tr}[(3\widehat{P}^{2} \cdot 2\widehat{P}^{3})(\widehat{H} - \widehat{\mu})] \qquad ($ $ = \text{tr}[(3\widehat{P}^{2} \cdot 2\widehat{P}^{3})(\widehat{H} - \widehat{\mu})] \qquad ($ $ = \text{tr}[(3\widehat{P}^{2} \cdot 2\widehat{P}^{3})(\widehat{H} - \widehat{\mu})] \qquad ($ $ = \text{tr}[(3\widehat{P}^{2} \cdot 2\widehat{P}^{3})(\widehat{H} - \widehat{\mu})] \qquad ($ $ = \text{tr}[(3\widehat{P}^{2} \cdot 2\widehat{P}^{3})(\widehat{H} - \widehat{\mu})] \qquad ($ $ = \text{tr}[(3\widehat{P}^{2} \cdot 2\widehat{P}^{3})(\widehat{H} - \widehat{\mu})] \qquad ($ $ = \text{tr}[(3\widehat{P}^{2} \cdot 2\widehat{P}^{3})(\widehat{H} - \widehat{\mu})] \qquad ($ $ = \text{tr}[(3\widehat{P}^{2} \cdot 2\widehat{P}^{3})(\widehat{H} - \widehat{\mu})] \qquad ($ $ = \text{tr}[(3\widehat{P}^{2} \cdot 2\widehat{P}^{3})(\widehat{H} - \widehat{\mu})] \qquad ($ $ = \text{tr}[(3P$		Let's defined a purified version of a trial density man	trix,
$\widetilde{\Omega} = \text{tr}[\widetilde{\rho}(\widehat{H} - \mu)] \qquad ($ $= \text{tr}[(3\widehat{\rho}^{2} - 2\widehat{\rho}^{3})(\widehat{H} - \widehat{\mu})] \qquad ($ $= \text{tr}[(3\widehat{\rho}^{2} - 2\widehat{\rho}^{3})\widehat{H}'] \qquad ($ $= \text{tr}[(3\widehat{\rho}^{2} - 2\widehat{\rho}^{3})\widehat{H}'] \qquad ($ $\text{where} \qquad ($ $\widehat{H}' = \widehat{H} - \mu \qquad ($ $(Gradient) \qquad (Gradient) $			(9)
$= \text{tr}[(3\hat{\rho}^{2} - 2\hat{\rho}^{3})(\hat{H} - \hat{\mu})] \qquad ($ $= \text{tr}[(3\hat{\rho}^{2} - 2\hat{\rho}^{3})\hat{H}'] \qquad ($ $\text{where} \qquad ($ $\hat{H}' = \hat{H} - \mu \qquad ($ $(\text{Gradient}) \qquad ($ $\delta \tilde{\Delta} = \text{tr}[3(\hat{\rho} + \hat{\rho} + \hat{\rho} + \hat{\rho})\hat{H}' - 2(\hat{\rho}^{3} + \hat{\rho} +$		The modified grand potential is then defined as	
$= \text{tr}[(3\hat{\rho}^{2} \cdot 2\hat{\rho}^{3}) \hat{H}']$ where $\hat{H}' = \hat{H} - \mu$ (Gradient) $\delta \hat{\Omega} = \text{tr}[3(\hat{\rho} \cdot s\hat{\rho} + s\hat{\rho}\hat{\rho}) \hat{H}' - 2(\hat{\rho}^{2} \cdot s\hat{\rho} + \hat{\rho} \cdot s\hat{\rho}\hat{\rho} + s\hat{\rho}\hat{\rho}^{2}) \hat{H}']$ $= \text{tr}[3(\hat{H}'\hat{\rho} + \hat{\rho}\hat{H}') \cdot s\hat{\rho} - 2(\hat{H}'\hat{\rho}^{2} + \hat{\rho}\hat{H}\hat{\rho} + \hat{\rho}^{2}\hat{H}') \cdot s\hat{\rho}]$ (\bigcirc equite shifts) Note that the gradient is defined as $\delta \hat{\Omega} = \text{tr}(\frac{3\hat{\Omega}}{3\hat{\rho}} \cdot s\hat{\rho}) = \sum_{ij} (\frac{3\hat{\Omega}}{3\hat{\rho}})_{ij} \cdot s\hat{\rho}_{ii}$ (comparing Eqs. (14) and (15),		$\widetilde{\Omega} = \text{tr}[\widetilde{P}(\widehat{H}-\mu)]$	(10)
where $\widehat{H}' = \widehat{H} - \mu$ (Gradient) $\widehat{S}\widetilde{\Delta} = \text{tr} \left[3(\widehat{\rho}\widehat{S}\widehat{\rho} + \widehat{S}\widehat{\rho}\widehat{\rho})\widehat{H}' - 2(\widehat{\rho}^{2}\widehat{S}\widehat{\rho} + \widehat{\rho}\widehat{S}\widehat{\rho} + \widehat{S}\widehat{\rho}\widehat{\rho}^{2} + \widehat{S}\widehat{\rho}\widehat{\rho}^{2})\widehat{H}' \right]$ $= \text{tr} \left[3(\widehat{H}'\widehat{\rho} + \widehat{\rho}\widehat{H}')\widehat{S}\widehat{\rho} - 2(\widehat{H}'\widehat{\rho}^{2} + \widehat{\rho}\widehat{H}\widehat{\rho}^{2} + \widehat{\rho}^{2}\widehat{H}')\widehat{S}\widehat{\rho} \right] $ (Outdie shifts) Note that the gradient is defined as $\widehat{S}\widetilde{\Delta} = \text{tr} \left(\frac{3\widetilde{\Omega}}{3\widehat{\rho}} \widehat{S}\widehat{\rho} \right) = \sum_{ij} \left(\frac{3\widetilde{\Omega}}{3\widehat{\rho}} \right)_{ij} \widehat{S}\widehat{\rho}_{ij} $ (Tomparing Eqs. (14) and (15),		$= tr[(3\hat{\rho}^{\frac{3}{2}}2\hat{\rho}^{3})(\hat{H}-\hat{\mu})]$	(11)
(Gradient) $\delta\widetilde{\Delta} = \text{tr} \left[3(\hat{\rho} \hat{s} \hat{\rho} + \hat{s} \hat{\rho} \hat{\rho}) \hat{H}' - 2(\hat{\rho}^{2} \hat{s} \hat{\rho} + \hat{\rho} \hat{s} \hat{\rho} \hat{\rho} + \hat{s} \hat{\rho} \hat{\rho}^{2}) \hat{H}' \right]$ $= \text{tr} \left[3(\hat{H}' \hat{\rho} + \hat{\rho} \hat{H}') \hat{s} \hat{\rho} - 2(\hat{H}' \hat{\rho}^{2} + \hat{\rho} \hat{H} \hat{\rho} + \hat{\rho}^{2} \hat{H}) \hat{s} \hat{\rho} \right] \qquad (\Theta \text{cyclic shifts})$ Note that the gradient is defined as $\delta\widetilde{\Delta} = \text{tr} \left(\frac{3\widetilde{\Omega}}{3\widehat{\rho}} \hat{s} \hat{\rho} \right) = \sum_{ij} \left(\frac{3\widetilde{\Omega}}{3\widehat{\rho}} \right) \hat{s} \hat{\rho}_{ij} \qquad (1)$ Comparing Eqs. (14) and (15),		$= \operatorname{tr}[(3\hat{\rho}^{\frac{2}{3}}2\hat{\rho}^{3})\hat{H}']$	(12)
$\delta\widetilde{\Omega} = \text{tr} \left[3(\hat{\rho} \hat{s} \hat{\rho} + \hat{s} \hat{\rho} \hat{\rho}) \hat{H}' - 2(\hat{\rho}^{\dagger} \hat{s} \hat{\rho} + \hat{\rho} \hat{s} \hat{\rho} \hat{\rho} + \hat{s} \hat{\rho} \hat{\rho}^{\dagger}) \hat{H}' \right]$ $= \text{tr} \left[3(\hat{H}' \hat{\rho} + \hat{\rho} \hat{H}') \hat{s} \hat{\rho} - 2(\hat{H}' \hat{\rho}^{\dagger} + \hat{\rho} \hat{H} \hat{\rho} + \hat{\rho}^{\dagger} \hat{H}) \hat{s} \hat{\rho} \right] \qquad (\Theta \text{oddie shifts})$ $\text{Note that the gnadient is defined as}$ $\delta\widetilde{\Omega} = \text{tr} \left(\frac{3\widetilde{\Omega}}{3\widehat{\rho}} \hat{s} \hat{\rho} \right) = \sum_{ij} \left(\frac{3\widetilde{\Omega}}{3\widehat{\rho}} \right) \hat{s} \hat{P}_{ji} \qquad (1)$ $\text{Comparing Eqs. (14) and (15)},$	0		(13)
$\delta\widetilde{\Omega} = \text{tr} \left[3(\hat{\rho} \hat{s} \hat{\rho} + \hat{s} \hat{\rho} \hat{\rho}) \hat{H}' - 2(\hat{\rho}^{\dagger} \hat{s} \hat{\rho} + \hat{\rho} \hat{s} \hat{\rho} \hat{\rho} + \hat{s} \hat{\rho} \hat{\rho}^{\dagger}) \hat{H}' \right]$ $= \text{tr} \left[3(\hat{H}' \hat{\rho} + \hat{\rho} \hat{H}') \hat{s} \hat{\rho} - 2(\hat{H}' \hat{\rho}^{\dagger} + \hat{\rho} \hat{H} \hat{\rho} + \hat{\rho}^{\dagger} \hat{H}) \hat{s} \hat{\rho} \right] \qquad (\Theta \text{updic shifts})$ $\text{Note that the gnadient is defined as}$ $\delta\widetilde{\Omega} = \text{tr} \left(\frac{3\widetilde{\Omega}}{3\widehat{\rho}} \hat{s} \hat{\rho} \right) = \sum_{ij} \left(\frac{3\widetilde{\Omega}}{3\widehat{\rho}} \right) \hat{s} \hat{\rho}_{ji} \qquad (1)$ $\text{Comparing Eqs. (14) and (15)},$		(Gradient)	
$\widehat{S\widetilde{\Omega}} = \operatorname{tr}(\widehat{\frac{\partial\widetilde{\Omega}}{\partial\widehat{\rho}}}\widehat{S\widehat{\rho}}) = \sum_{ij} (\widehat{\frac{\partial\widetilde{\Omega}}{\partial \rho}})_{ij} \widehat{SP}_{ji} $ $Comparing Eqs. (14) and (15), $		$8\widetilde{\Omega} = \text{tr} \left[3(\hat{\rho}\hat{s}\hat{\rho} + \hat{s}\hat{\rho}\hat{\rho}) \hat{H}' - 2(\hat{\rho}^{\dagger}\hat{s}\hat{\rho} + \hat{\rho}\hat{s}\hat{\rho}\hat{\rho} + \hat{s}\hat{\rho}\hat{\rho}^{\dagger}) \hat{H}' \right]$ $= \text{tr} \left[3(\hat{H}'\hat{\rho} + \hat{\rho}\hat{H}') \hat{s}\hat{\rho} - 2(\hat{H}'\hat{\rho}^{\dagger} + \hat{\rho}\hat{H}\hat{\rho} + \hat{\rho}^{\dagger}\hat{H}) \hat{s}\hat{\rho} \right]$	(14)
Comparing Egs. (14) and (15),	7	Note that the gradient is defined as	
	1. 3.00	$\widehat{S}\widetilde{\Omega} = \operatorname{tr}(\widehat{\beta}\widetilde{\Omega} \widehat{S}\widehat{\rho}) = \sum_{ij} (\widehat{\beta}\widetilde{\Omega})_{ij} \widehat{S}P_{ji}$	(15)
$\frac{3\tilde{\Omega}}{3\hat{\rho}} = 3(\hat{H}\hat{\rho} + \hat{\rho}\hat{H}') - 2(\hat{H}\hat{\rho}^2 + \hat{\rho}\hat{H}\hat{\rho} + \hat{\rho}^2\hat{H}') \tag{1}$		Comparing Egs. (14) and (15),	
		$\frac{\partial \widetilde{\Omega}}{\partial \widehat{\rho}} = 3(\widehat{H}\widehat{\rho} + \widehat{\rho}\widehat{H}') - 2(\widehat{H}\widehat{\rho}^2 + \widehat{\rho}\widehat{H}\widehat{\rho} + \widehat{\rho}^2\widehat{H}')$	(16)

(Theorem) The unconstrained minimum of I gives the constrained ground state of D.

(Stationarity)

At the constrained minimum, P satisfies the idempotency condition, $\hat{P}^2 = \hat{P}$, and also $\hat{P} = \Theta(-\hat{H}')$ commutes with \hat{H}' . Therefore,

$$\frac{\partial \widetilde{\Omega}}{\partial \widehat{\rho}} = 6 \widehat{\rho} \widehat{H}' - 6 \widehat{\rho}^2 \widehat{H}' = 0$$

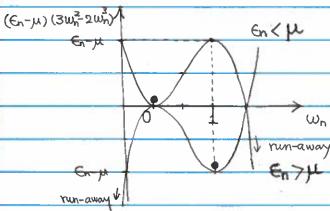
(minimum)

Let the trial ô be expanded with the energy eigenstates, (17)

$$\widehat{\rho} = \sum_{n} |n\rangle w_n \langle n|$$

Within this variational space (which contains the ground state),

$$\widetilde{\Omega} = \sum_{n} (\xi_{n} - \mu) (3\omega_{n}^{2} - 2\omega_{n}^{3})$$



The minimum of this function is w

$$\omega_n = \begin{cases} 1 & (\forall \in_n < \mathcal{M}) \\ 0 & (\forall \in_n > \mathcal{M}) \end{cases}$$

which is a minimum, with the correst ground-state value,

(19)

(single minimum)
Since $\widetilde{\Sigma}$ is a cubic function of $\widehat{\rho}$, along any line-

minimization direction, there can be only one minimum.

(run-away solution)

There are run-away solutions, such as

$$\omega_{n} = \begin{cases} +\infty & (\forall \epsilon_{n} < \mu) \\ -\infty & (\forall \epsilon_{n} > \mu) \end{cases}$$

in the variational space (17), because of the cubic polynomial.

·:		6
0 -	Localization algorithm	
	With exponential accuracy, Pij can be approximated as	
	$P_{ij} = 0 (\forall R_{ij} > R_c)$	(20)
	where Rij is the distance between atoms the basis orbital i and j belong to, and Re is the cut-off length.	
*	M:m: ZA	
	Minimize $\widetilde{\Omega} = tc[(3\hat{\rho}^2 2\hat{\rho}^3)(\hat{H} - \mu)]$	(21)
	with respect to Pij with constraint	
	$P_{ij} = 0 (\forall R_{ij} > R_{c})$	(22)
	using the conjugate gradient algorithm with gradient	
	$\frac{\partial \widehat{C}}{\partial \widehat{\rho}} = 3(\widehat{H}\widehat{\rho} + \widehat{\rho}\widehat{H}') - 2(\widehat{H}\widehat{\rho}^2 + \widehat{\rho}\widehat{H}\widehat{\rho}^2 + \widehat{\rho}^2\widehat{H}')$	(23)
		200 200 200

On the constrained minimization, Eq.(7)

Minimize, with respect to
$$\hat{P}$$
,

 $\Omega = \text{tr} \left[\hat{P}(\hat{H}-\mu) \right]$ (24)

with idempotency constraint $\hat{\rho}^2 - \hat{\rho} = 0 \tag{25}$

To solve this problem, we introduce Lagrange multipliers
$$\Omega' = \operatorname{tr}\left[\hat{\rho}(\hat{H} - \mu) - \hat{\Lambda}(\hat{\rho}^2 \hat{\rho})\right] \tag{26}$$

The solution is stationary with respect to both $\hat{\rho}$ and $\hat{\Lambda}$, $\frac{\partial \Omega'}{\partial \hat{\Lambda}} = \hat{\rho}^2 - \hat{\rho} = 0$ (27)

Functional derivative with respect to
$$\hat{\rho}$$
 is $8\Omega' = \text{tr}[(\hat{H} - \mu) \hat{S}\hat{\rho} - \hat{\Lambda}(\hat{\rho}\hat{S}\hat{\rho} + \hat{S}\hat{\rho}\hat{\rho} - \hat{S}\hat{\rho})]$

=
$$\operatorname{tr}\left[(\hat{H}-\mu)\hat{S}\hat{\rho}-(\hat{\Lambda}\hat{\rho}+\hat{\rho}\hat{\Lambda}-\hat{\Lambda})\hat{S}\hat{\rho}\right]$$

$$\frac{\partial \Omega'}{\partial \hat{\rho}} = \hat{H} - \mu - (\hat{\Lambda} \hat{\rho} + \hat{\rho} \hat{\Lambda} - \hat{\Lambda}) = 0$$
 (28)

Let's examine the solution in terms of the eigenstates of $\hat{\rho}$, $\langle n| \times \text{Eq.}(27) \times |n\rangle$

$$\rho_n^2 - \rho_n = \rho_n (\rho_n - 1) = 0$$

$$\therefore P_n = 1 \text{ or } 0$$

<n1 × Eq. (27) × In>

$$H_{nn}-\mu = \Lambda_{nn} (2P_n-1)$$

$$\therefore \Lambda_{nn} = \begin{cases} H_{nn} - \mu & (P_n = 1) \\ \mu - H_{nn} & (P_n = 0) \end{cases}$$

